

Status of Extended Chemistry Climate Models

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16 June 2004

Describe Model Components

Evaluation with Observations

Future use of Occultation Data

Extended Chemistry Climate Models...

Climate Model (Atm)

Tropospheric focus

Typically 0-40km

Little or no chemistry

Ocean

Land Surface

Sea Ice

3-D Extended Chemistry Climate Models

Institution
NASA GISS
CMAM
MPI ECHAM
MPI HARMONIA
NOAA GFDL
NASA GSFC
University Illinois
University of Reading
University of Cambridge
Imperial College
UKMO Met Office
Freie Universitat, Berlin
NCAR WACCM

C/C @ NCAR; WACCM Investigators

- ACD: **Rolando Garcia (PI)**
 - Doug Kinnison, Dan Marsh, Stacy Walters, Anne Smith, JF Lamarque, Aimee Merkel, Jaga Beres, Bill Randel, Laura Pan, Cyndi Nevison, Louisa Emmons, Peter Hess, John Orlando, Geoff Tyndall
- CGD: **Byron Boville (PI)**
 - Fabrizio Sassi, Andrew Gettelman, Phil Rasch, CAM3 colleagues etc...
- HAO: **Ray Roble (PI)**
 - Stan Solomon, Maura Hagan, Hanli Lui, Ben Foster

Extending the Community Atmospheric Model

To form WACCM...

- Parameterization of non-LTE IR (15 μm band of CO₂ above 70 km) merged with CCSM IR parameterization (below 70 km)
- Short wave heating rates due to absorption of radiation shortward of 200 nm and chemical potential heating
- Gravity Wave parameterization extended upward, includes dissipation by molecular viscosity
- Effects of dissipation of momentum and heat by molecular viscosity (dominant above 100 km)
- Diffusive separation of atmospheric constituents above about 90 km
- Simplified parameterization of ion drag
- Finite-volume dynamics (Lin and Rood, 1996)
- Modified cloud water and near-IR parameterizations for more accurate seasonal cycle of temperature at tropopause

Model Chemistry - 50 Species Mechanism

Long-lived Species: (19-species) - Explicit Forward Euler

Misc:	CO ₂ , CO, CH ₄ , H ₂ O, N ₂ O, H ₂ , O ₂
CFCs:	CCl ₄ , CFC-11, CFC-12, CFC-113
HCFCs:	HCFC-22
Chlorocarbons:	CH ₃ Cl, CH ₃ CCl ₃ ,
Bromocarbons:	CH ₃ Br
Halons:	H-1211, H-1301
Constant Species:	N ₂ , N(² D)

Short-lived Species: (31-species) - Implicit Backward Euler*

O _x :	O ₃ , O, O(¹ D)
NO _x :	N, NO, NO ₂ , NO ₃ , N ₂ O ₅ , HNO ₃ , HO ₂ NO ₂
ClO _x :	Cl, ClO, Cl ₂ O ₂ , OCIO, HOCl, HCl, ClONO ₂ , Cl ₂
BrO _x :	Br, BrO, HOBr, HBr, BrCl, BrONO ₂
HO _x :	H, OH, HO ₂ , H ₂ O ₂
CH ₄ derivatives:	CH ₂ O, CH ₃ O ₂ , CH ₃ OOH

* Non-linear system of equations are solved using a Newton Raphson iteration technique; uses sparse matrix techniques; Sandu et al, *J. Comp. Phys.*, 129, 101-110, 1996.

Model Chemistry - 106 Species Mechanism (219 Thermal; 18 Het.; 71 photolytic)

Additional Surface Source Gases (13 additional) ...

NHMCs:

CH₃OH,
C₂H₆, C₂H₄, C₂H₅OH, CH₃C = HO
C₃H₈, C₃H₆, CH₃COCH₃ (Acetone)
C₄H₈ (BIGENE), C₄H₈O (MEK)
C₅H₈ (Isoprene), C₅H₁₂ (BIGALK)
C₇H₈ (Toluene)
C₁₀H₁₆ (Terpenes)

Radicals:

Approx. 45 additional species.

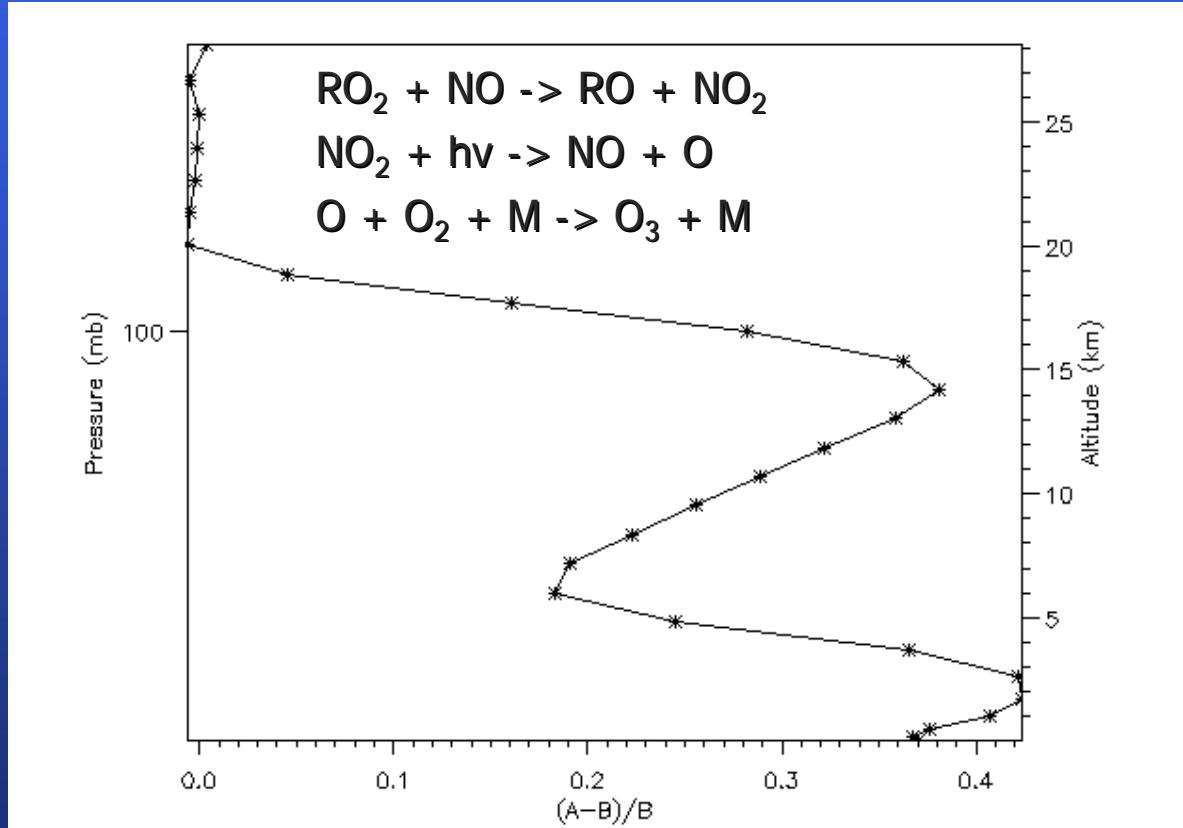
Include:

Detailed 3D (lat/lon/time) emission inventories of natural and anthropogenic surface sources

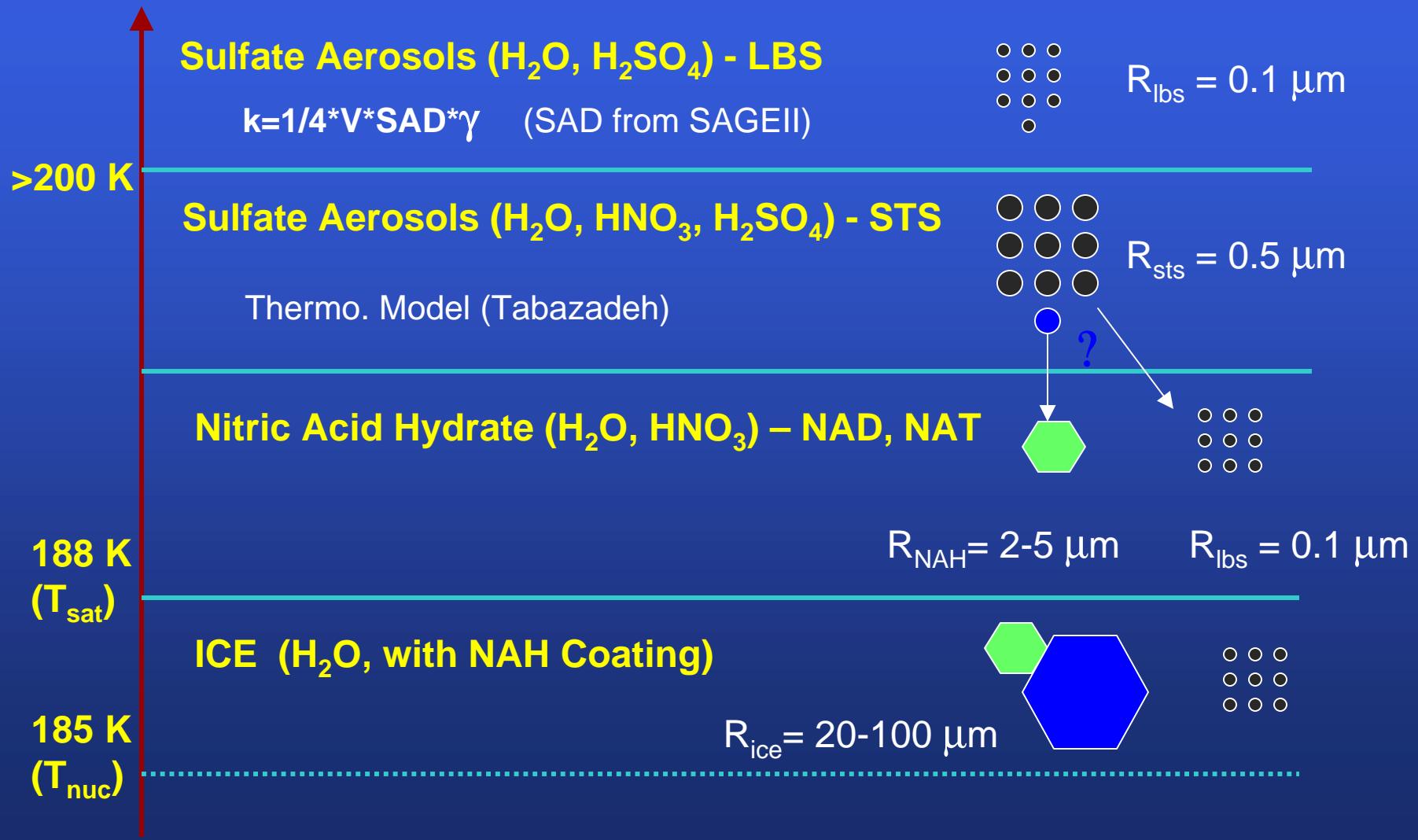
Dry and wet deposition of soluble species
Lightning and Aircraft production of NOx

Comparison of Mechanisms (106 - 50 / 50)

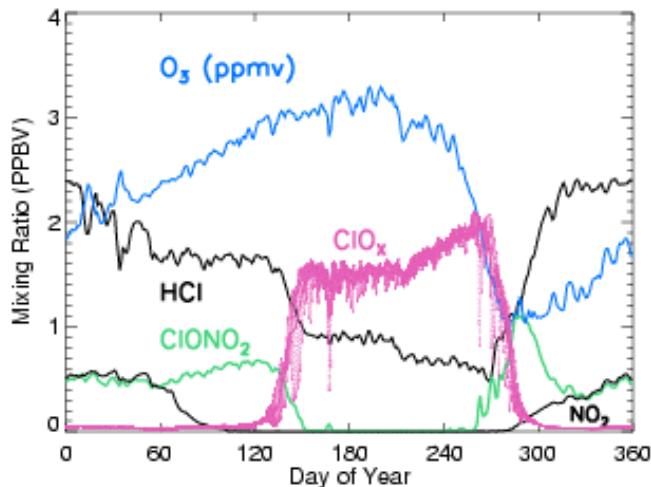
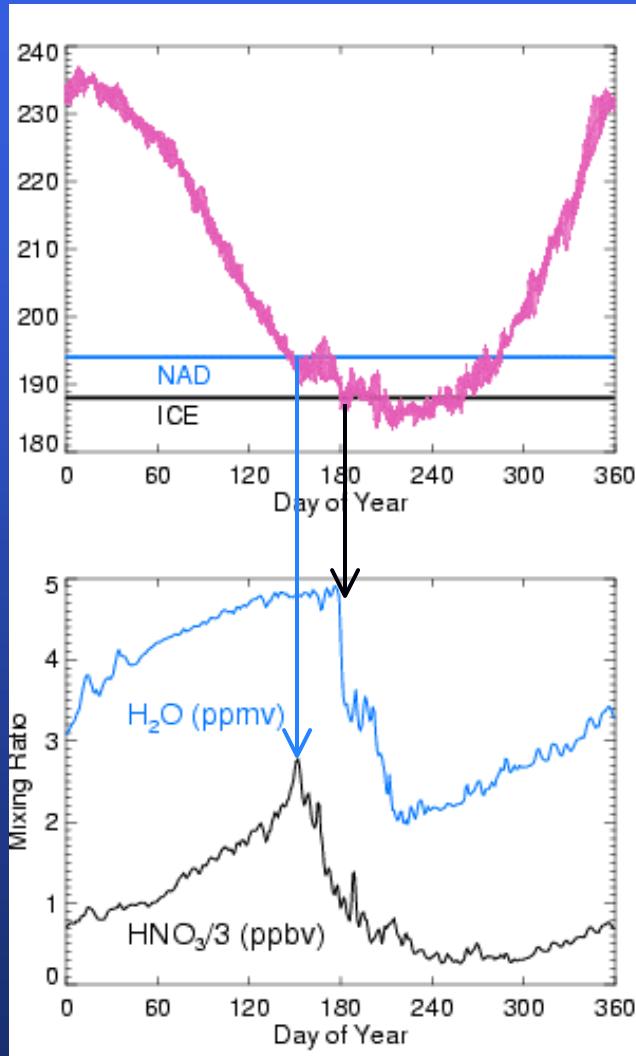
Ozone change in tropics



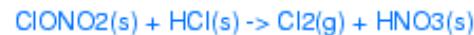
Model Chemistry - Heterogeneous Processes



Polar Chemistry example...



Activation in Winter/Spring



Ozone Depletion in Spring



Model Chemistry - Photolytic Processes

Photolysis: e.g., $O_2 + h\nu \rightarrow O(^3P) + O(^1D)$

$$\frac{d[O_2]}{dt} = J_{O_2} [O_2]$$

$$J_{O_2}(p) = \sum F_{\text{exo}}(\lambda, t) \times N_{\text{flux}}(p, \lambda) \times \sigma(\lambda) \times \phi(\lambda)$$

Inline (34 Bins)

LUT (122 Bins)

121 nm

- J_{O_2} Lyman Alpha
- J_{O_2} SRB
- J_{NO} SRB
- $\sigma \times \phi$ of ~15 species
- N_{flux} (p, λ) is funct. (O_3, O_2)

200 nm

- N_{flux} is based on TUV (Madronich)
- RSF (p, λ) is function of (Col. O_3 ; Zenith Angle, Albedo)
- $\sigma \times \phi$ is function of (T, p)

750 nm

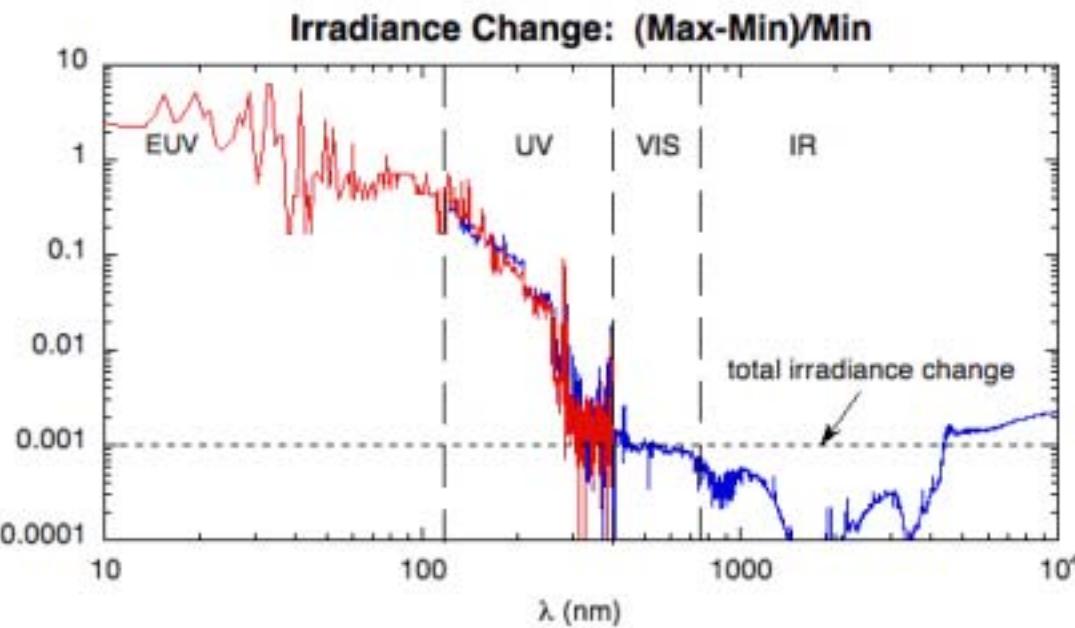
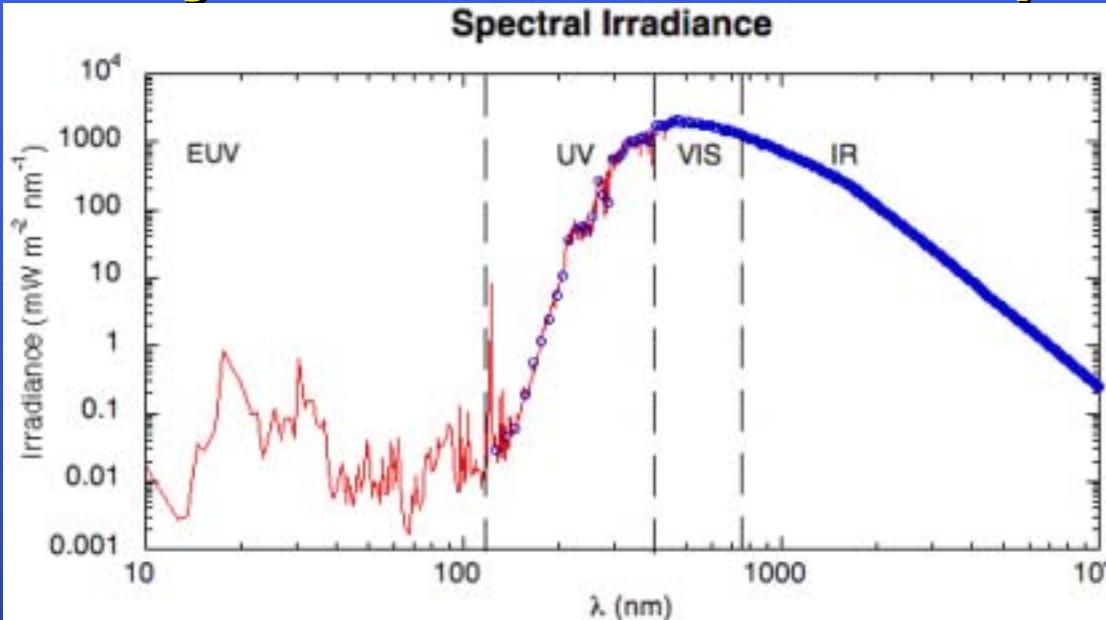
CAM3 SW Heating rates

← Heating and
Photolysis rates →

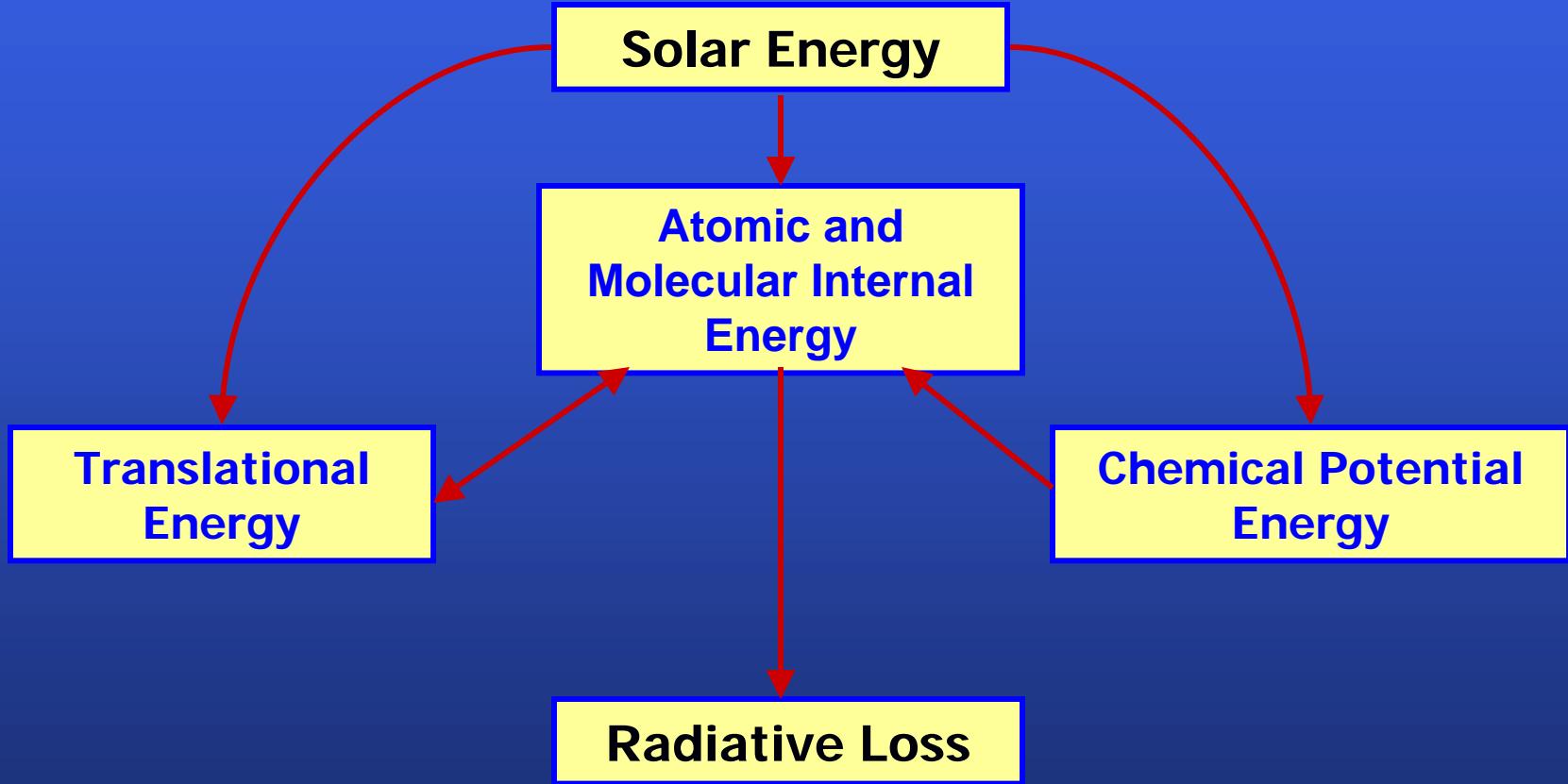
Solar Cycle Studies: Model Input

Spectral composite
courtesy of:

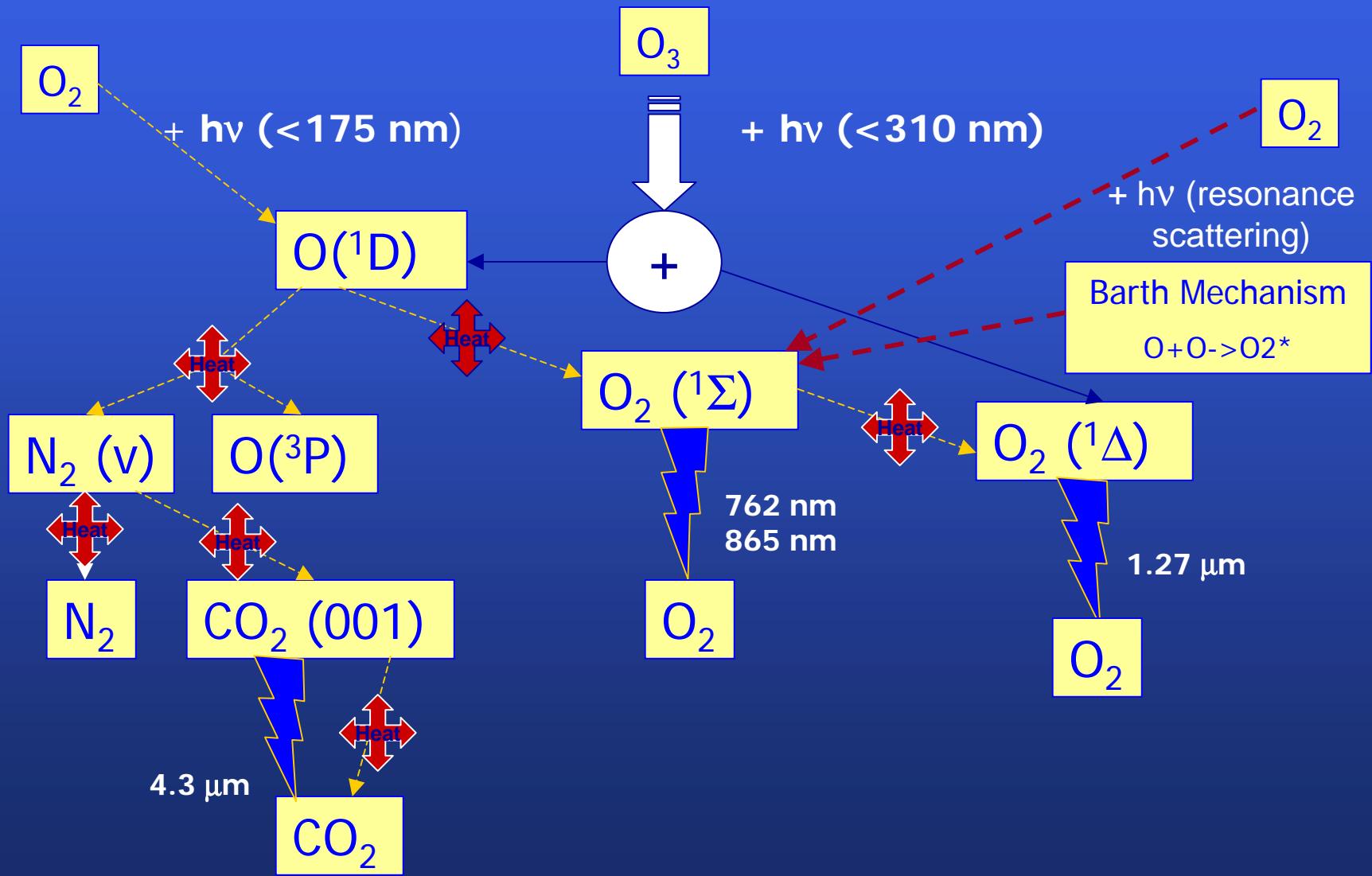
Judith Lean (NRL)
and
Tom Woods (CU/LASP)



Heating Rate Approach



Heating Rate Approach Cont...

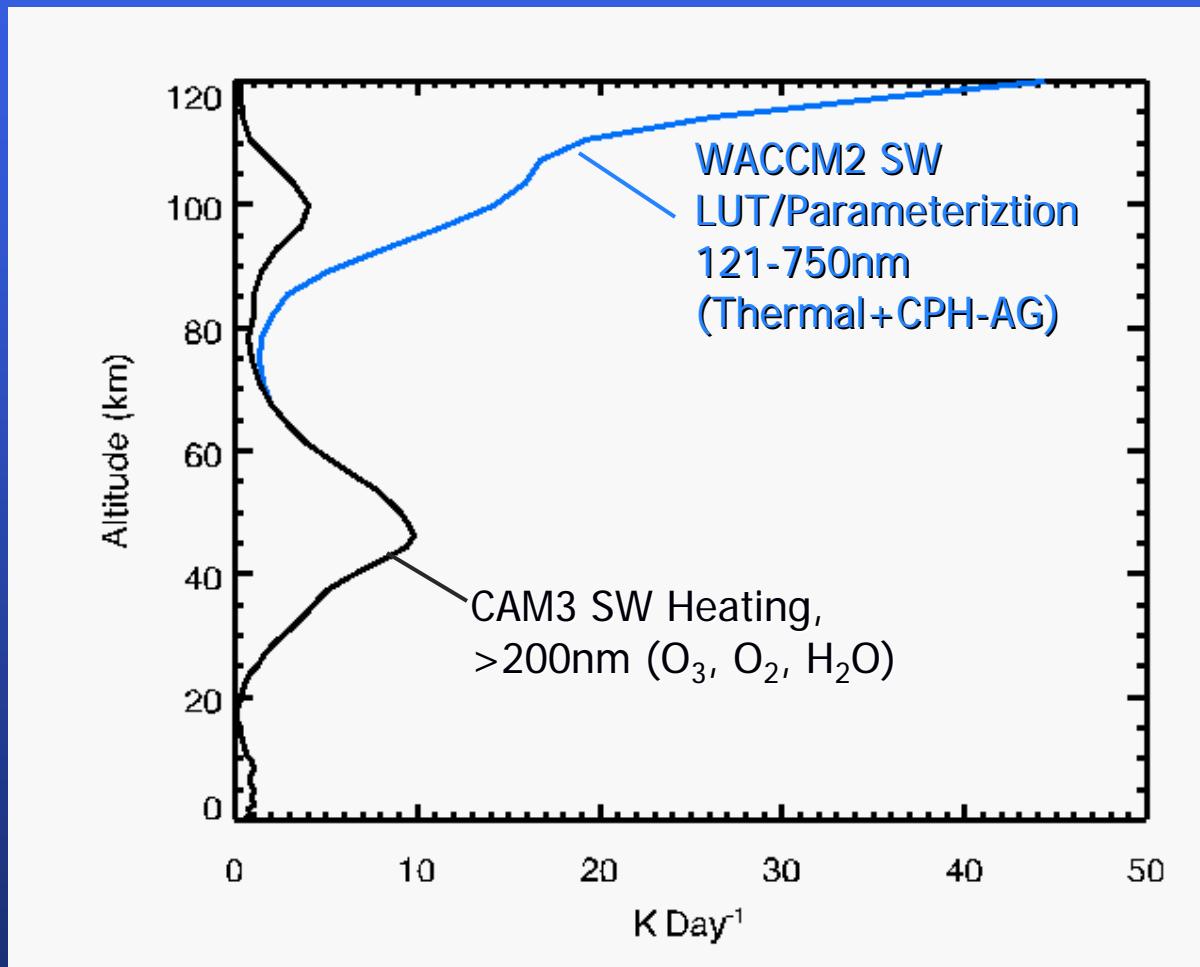


Chemical Potential Heating

Chemical Reactions	Kcal/mole
$O + O_3 \Rightarrow 2O_2$	-93.65
$O + O + M \Rightarrow O_2 + M$	-119.40
$O + OH \Rightarrow H + O_2$	-16.77
$O + HO_2 \Rightarrow OH + O_2$	-53.27
$H + O_2 + M \Rightarrow HO_2 + M$	-49.10
$O + O_2 + M \Rightarrow O_3 + M$	-25.47
$H + O_3 \Rightarrow OH + O_2$	-76.90
$HO_2 + NO \Rightarrow NO_2 + OH$	-7.83
$HO_2 + O_3 \Rightarrow OH + 2O_2$	-28.29
$HO_2 + HO_2 \Rightarrow H_2O_2 + O_2$	-39.58
$OH + O_3 \Rightarrow HO_2 + O_2$	-39.91
$NO + O_3 \Rightarrow NO_2 + O_2$	-47.74
$NO_2 + O \Rightarrow NO + O_2$	-45.91
$OH + HO_2 \Rightarrow H_2O + O_2$	-70.61
$H + HO_2 \Rightarrow H_2 + O_2$	-55.68

Mlynczak and Solomon

Heating Rate Approach (WACCM2)



NO_x Production from E-Region Ion Chemistry Included in WACCM2

Ion species:

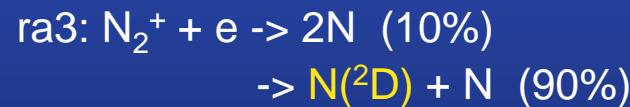
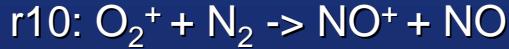
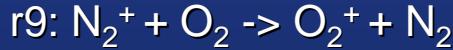
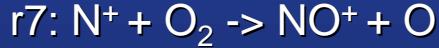
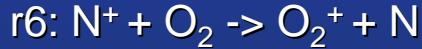
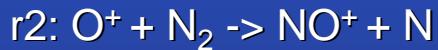
N₂⁺, O₂⁺, N⁺, O⁺, NO⁺, and e

EUV, Auroral, SPE's, GCR

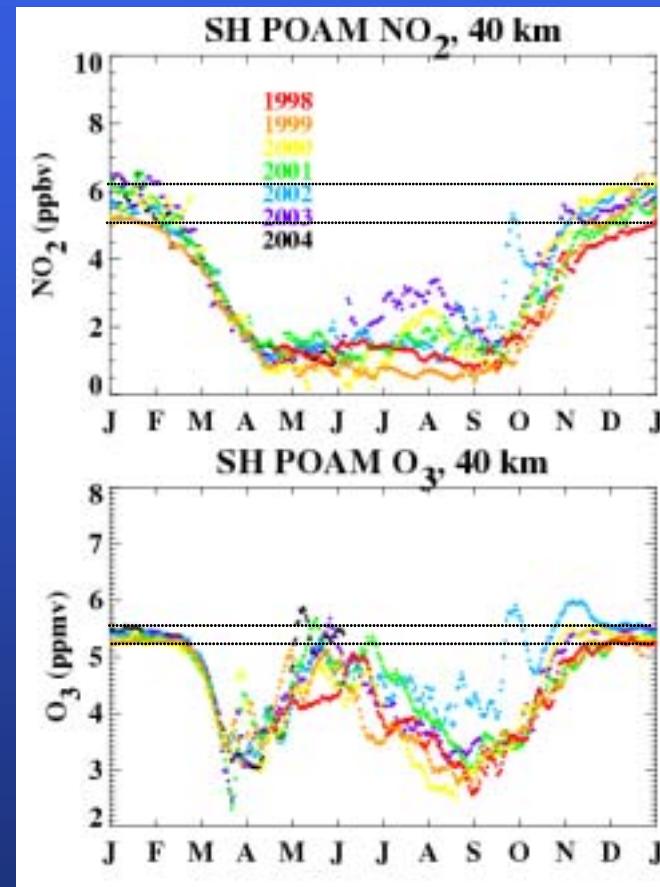
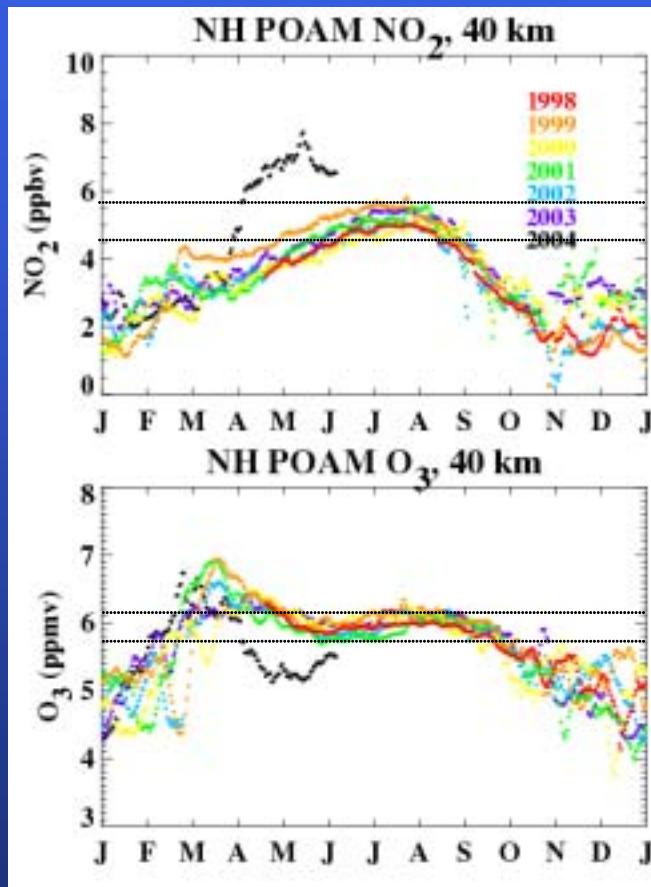
Photon / Photoelectron processes with
O, N, O₂, N₂

Approx. 25 reactions...

reactions:



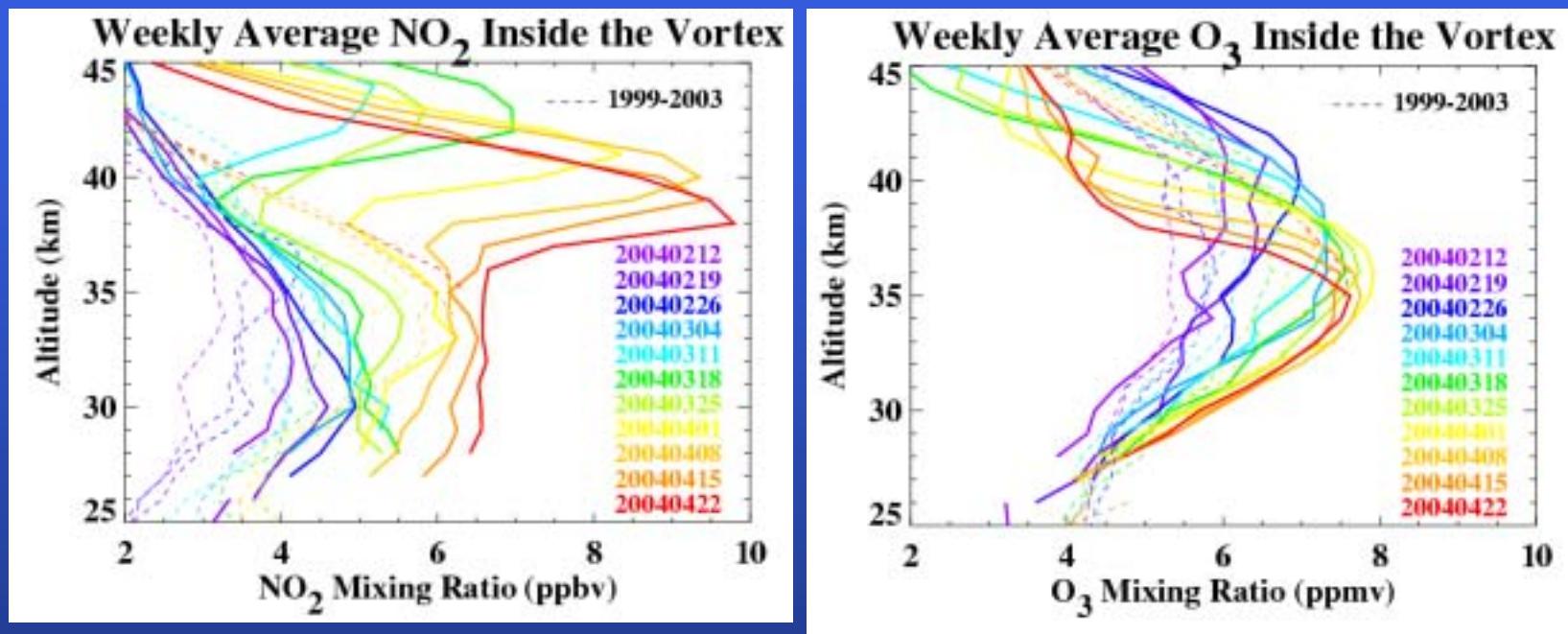
Interannual variability in POAM NO₂ exceeds 15% even in summer; Variability in summertime Ozone ~5-7%.



Some of the variability can be attributed to **ENERGETIC PARTICLE EFFECTS**.

How significant are the errors in 3D simulations and trend analyses when energetic particle effects are ignored?

Unprecedented high NO_2 descends inside the NH vortex in Mar-Apr 2004: Corresponds to unprecedented low O_3



Solid lines: Weekly averages in 2004

Dotted lines: Weekly averages including data from 1999-2003

NO_x enhancements and O_3 decreases are due to ENERGETIC PARTICLE PRODUCTION of mesospheric NO, which descends to the stratosphere and catalytically destroys O_3 .

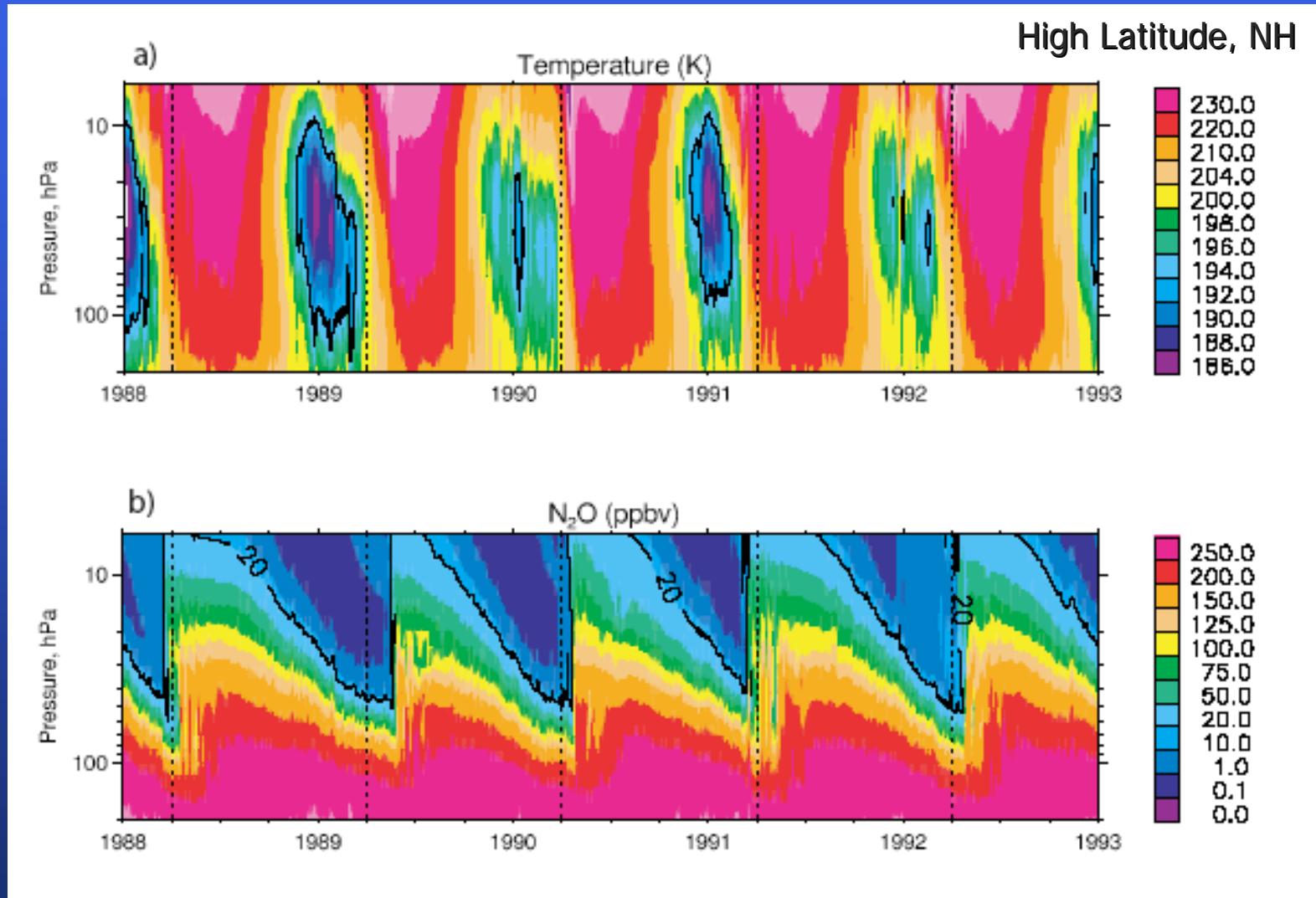
Describe Model Components

Evaluation with Observations

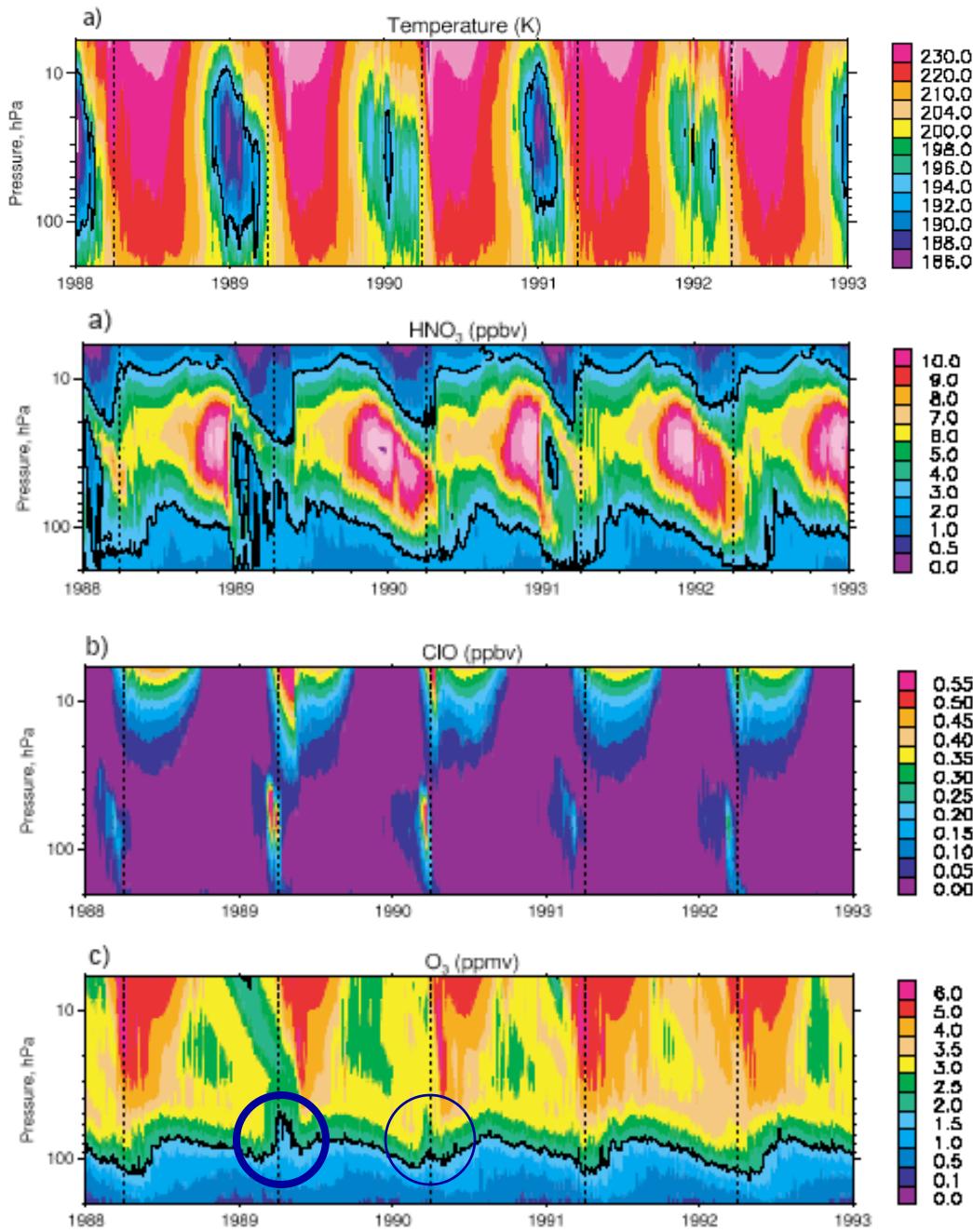
Future use of Occultation Data

Interannual Variability

Interannual Variability - No one year is the same!



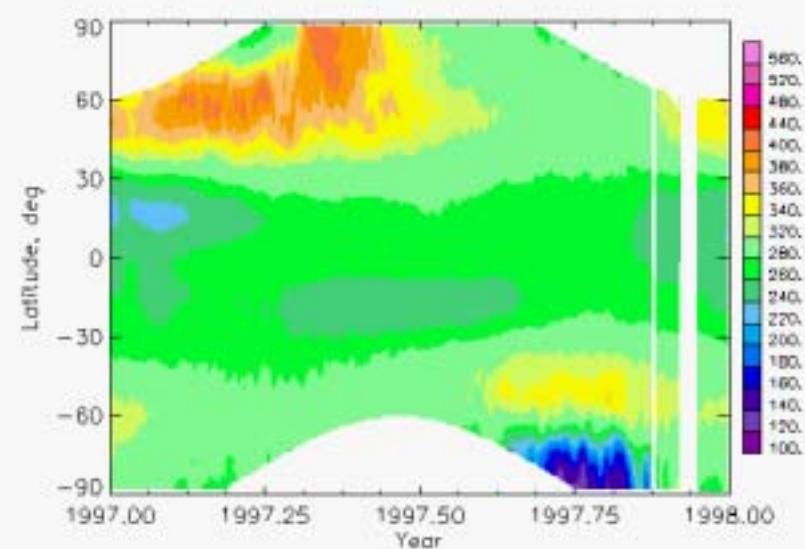
NH Chemical Ozone Loss



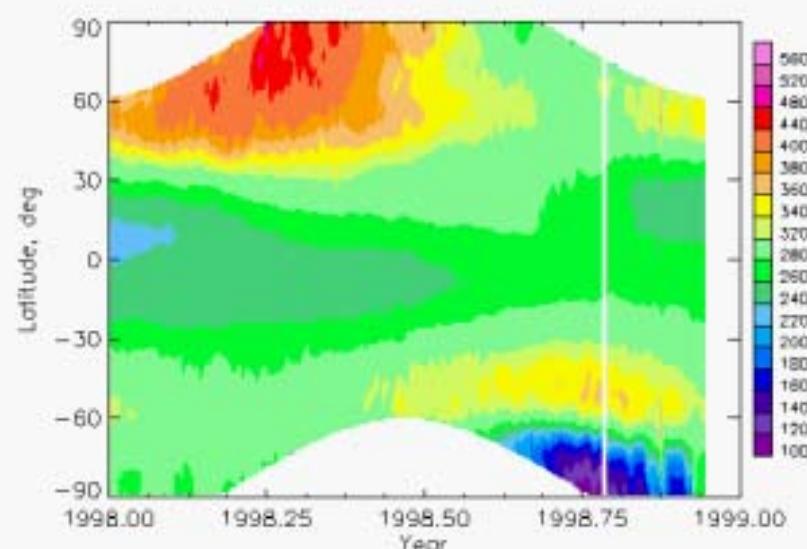
Sassi, Kinnison, Boville, Garcia, and Roble, The effect of ENSO on the dynamical, thermal and chemical structure of the middle atmosphere, *J. Geophys. Res.*, in review, 2004

Total Column Ozone (Data)

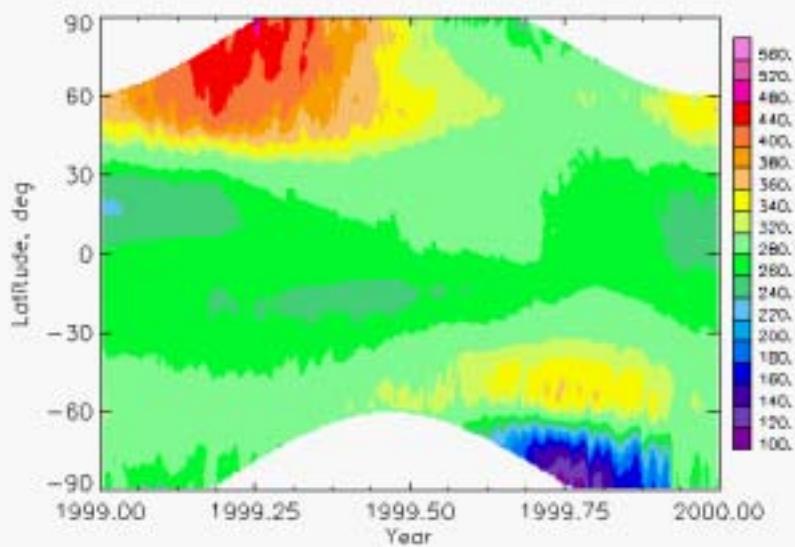
EPTOMS 1997



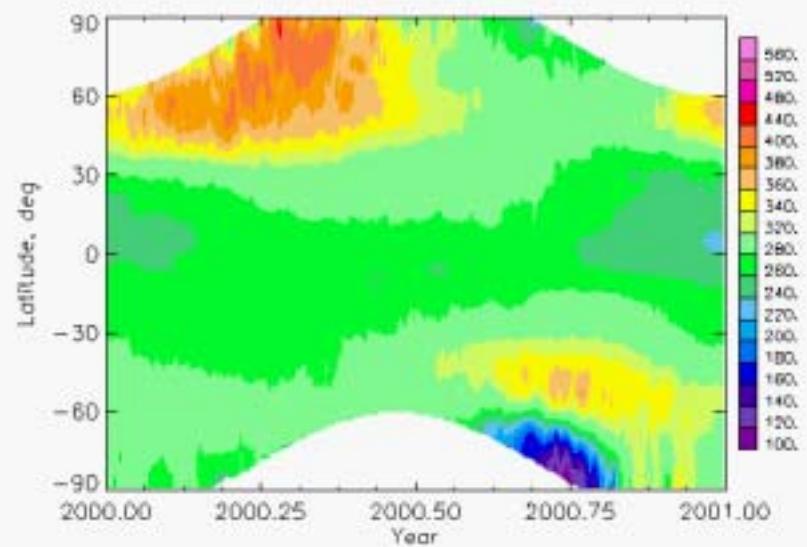
EPTOMS 1998



EPTOMS 1999



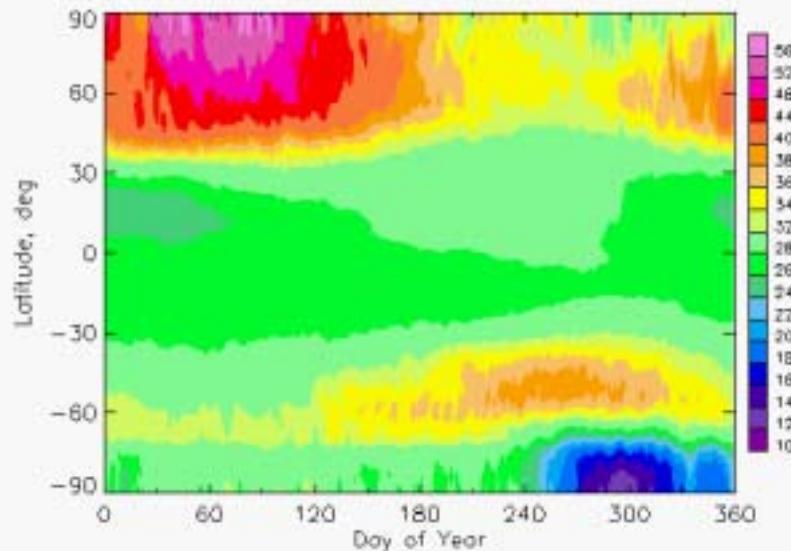
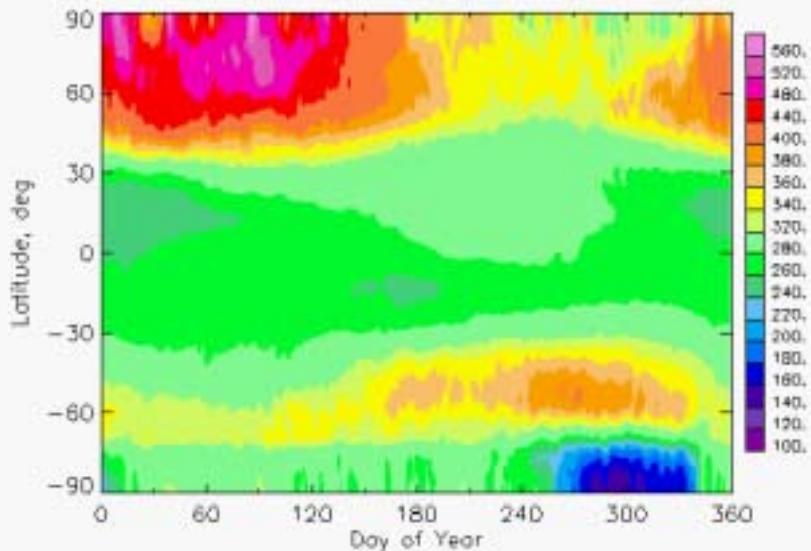
EPTOMS 2000



Total Column Ozone (WACCM2)

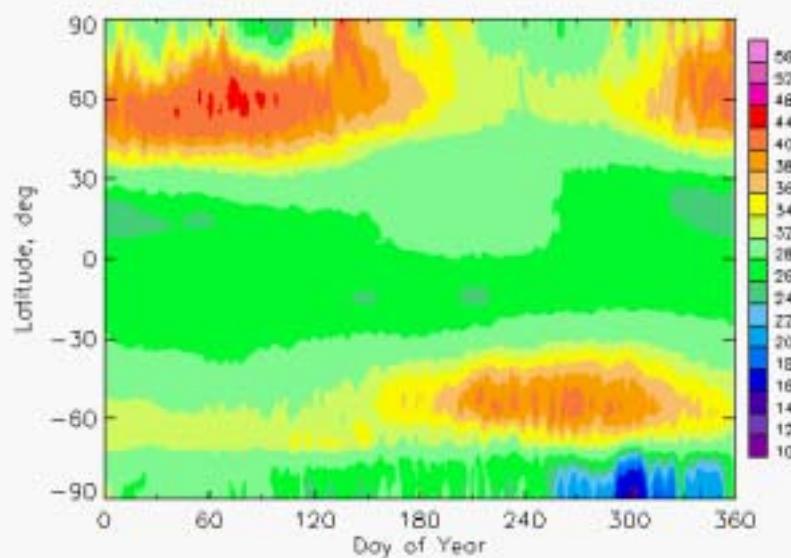
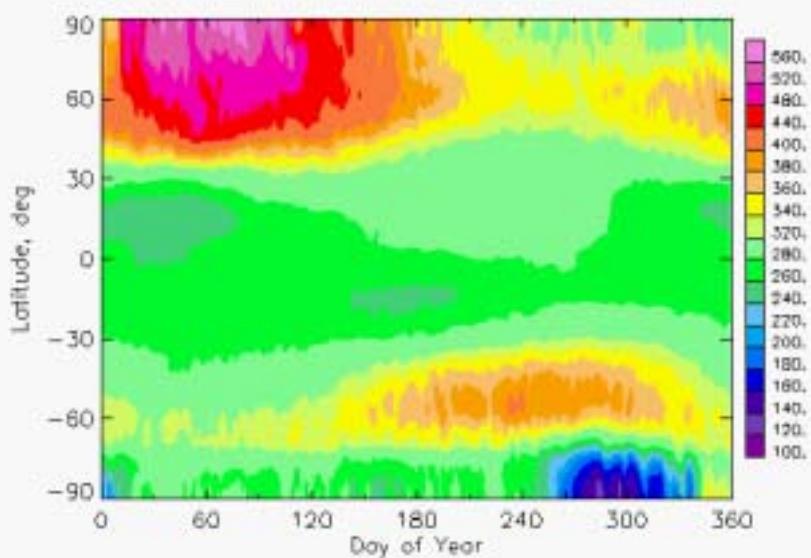
WACCM2 year 2

WACCM2 year 3



WACCM2 year 4

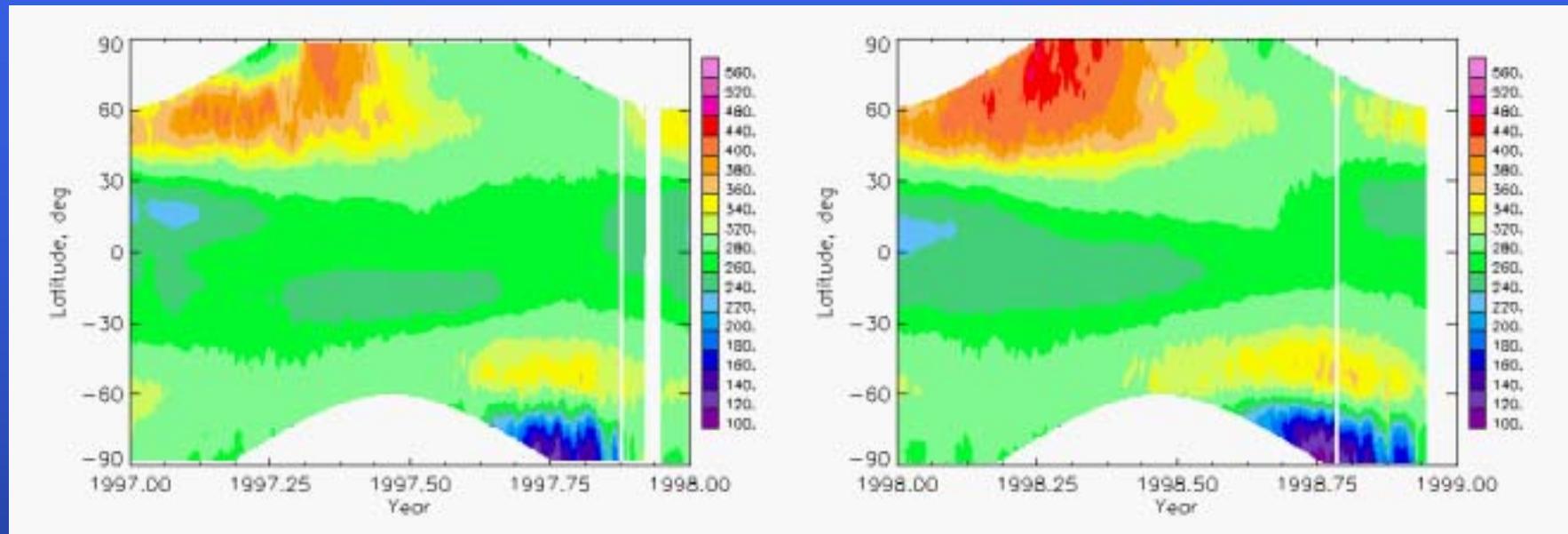
WACCM2 year 5



Total Column Ozone (WACCM2, EPTOMS)

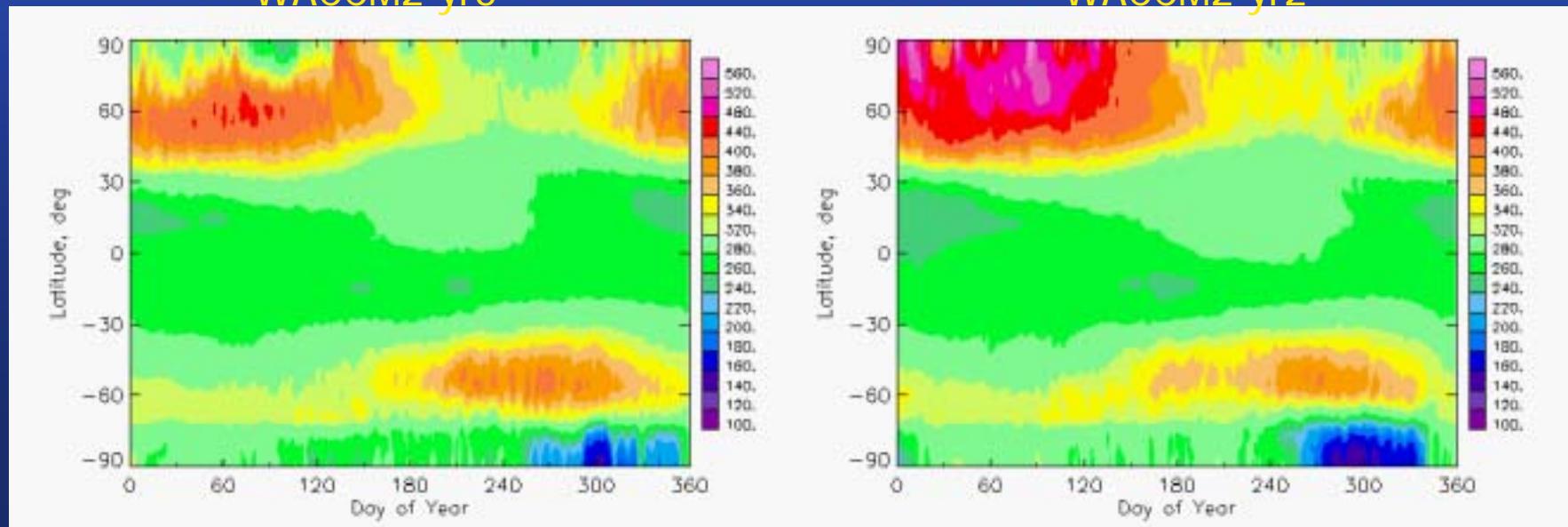
EPTOMS 1997

EPTOMS 1998

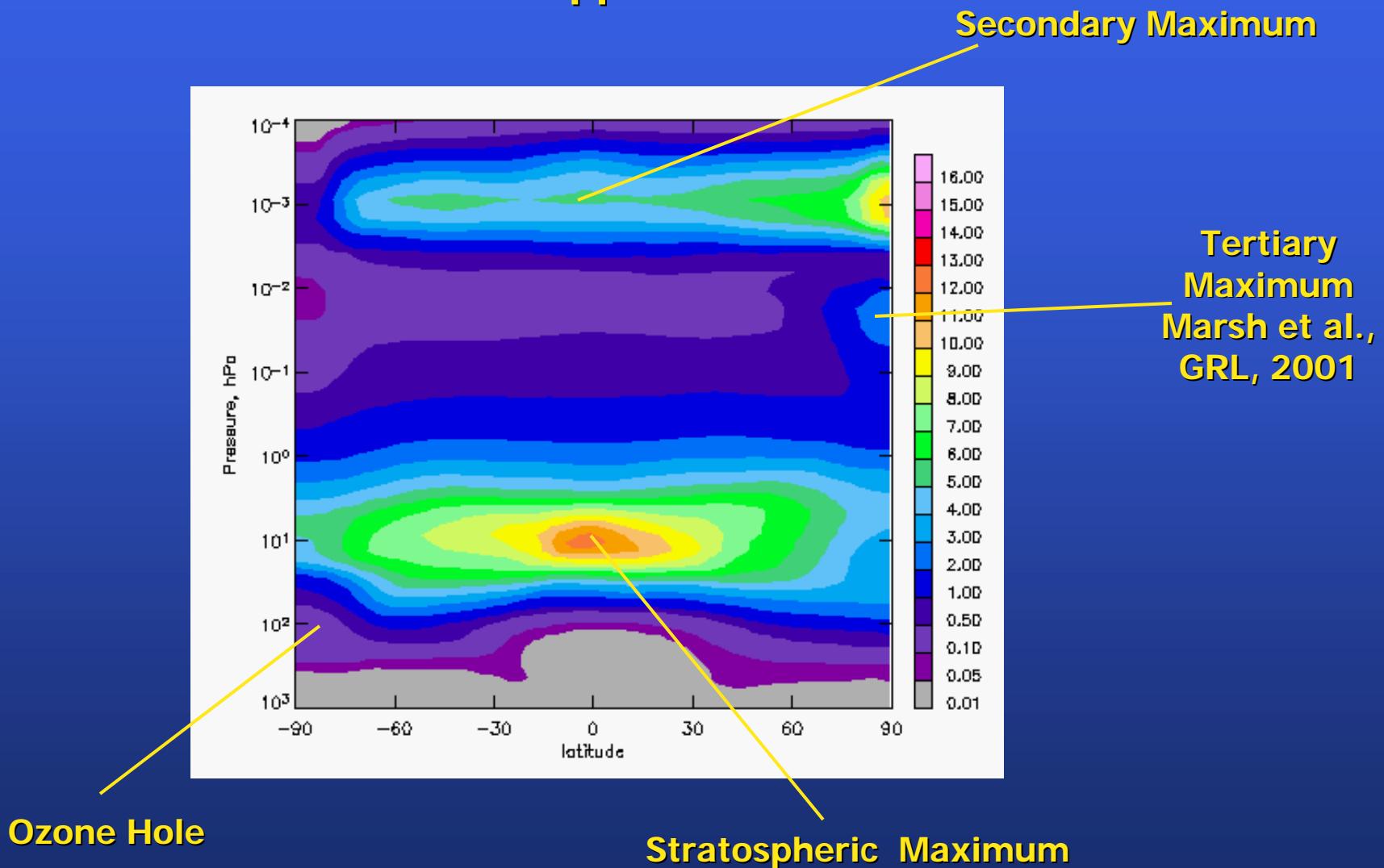


WACCM2 yr5

WACCM2 yr2



Ozone, October ppmv



WACCM/Occultation Ozone Comparisons

L. Harvey and C. Randall, LASP

Monthly Mean Climatology

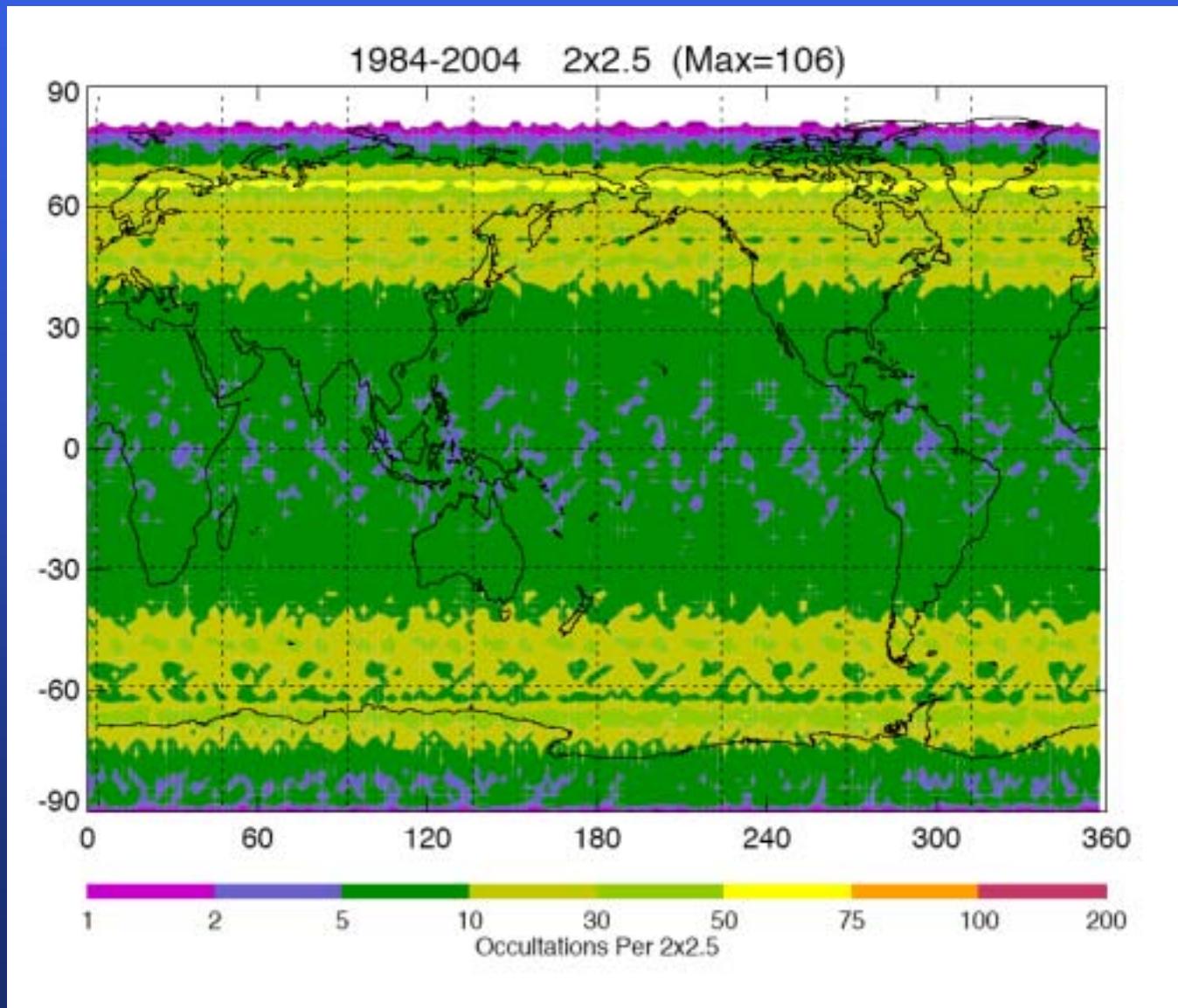
2° (longitude) x 2.5° (latitude) Grid
4° (longitude) x 5° (latitude) Grid

Occultation Data: SAGE II, III (1984-Present)
POAM II, III (1994-Present)
ILAS (1996-1997)
HALOE (1991-Present)

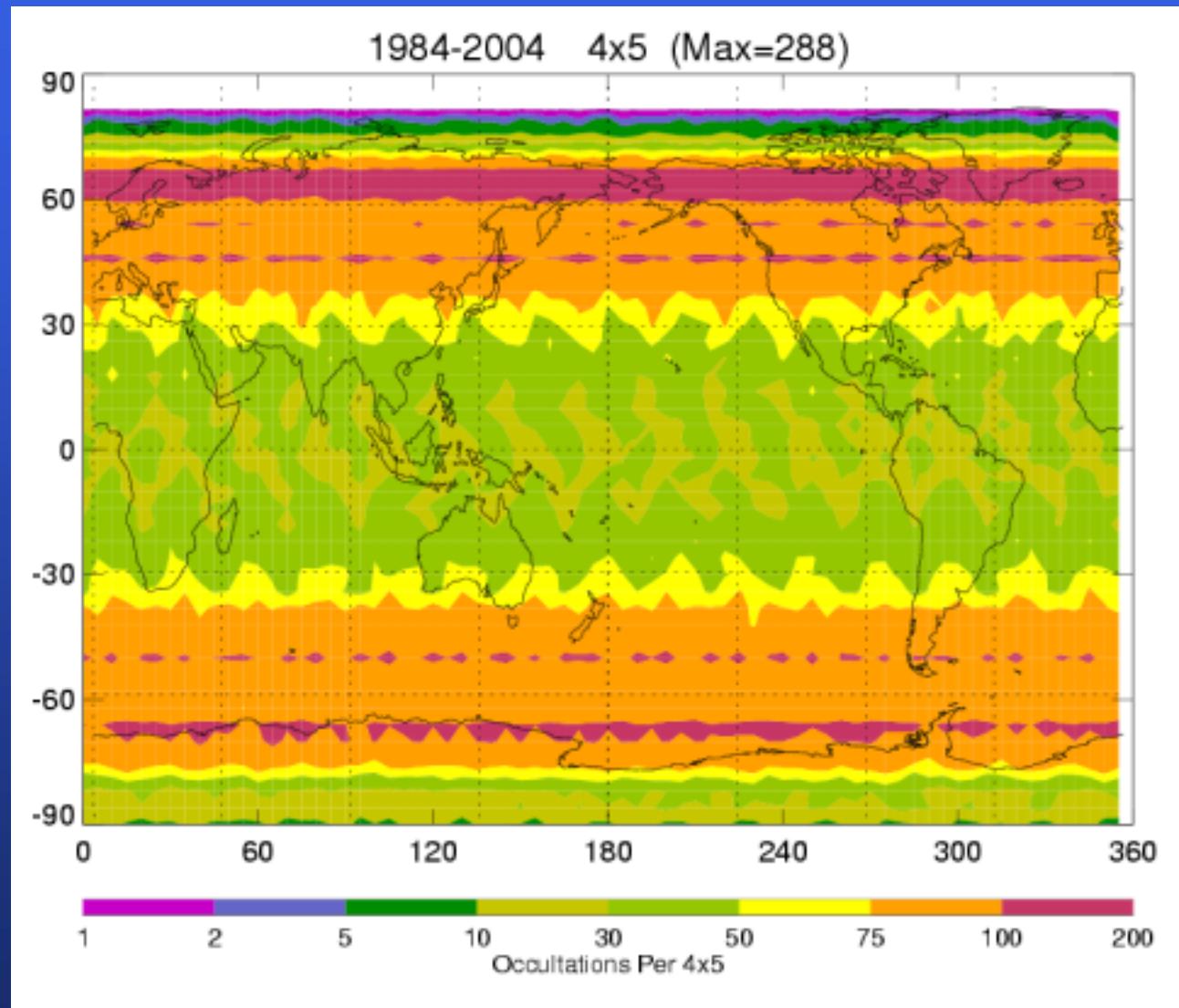
Species: O₃, CH₄, NO_x, HNO₃, H₂O

Also... Randel UARS Climatology

O₃, Occultation Statistics, 2x2.5

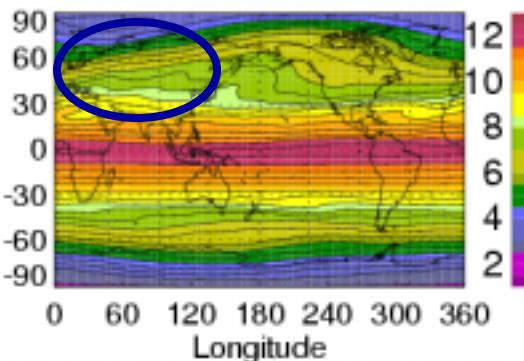


O₃, Occultation Statistics, 4x5

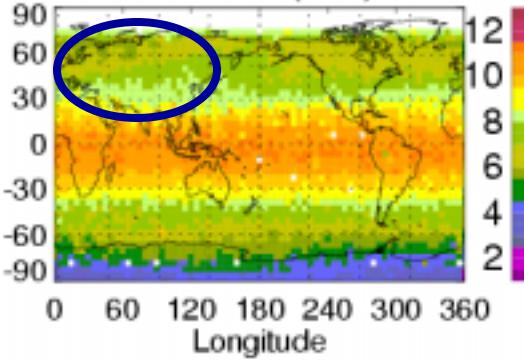


March 10 hPa Ozone

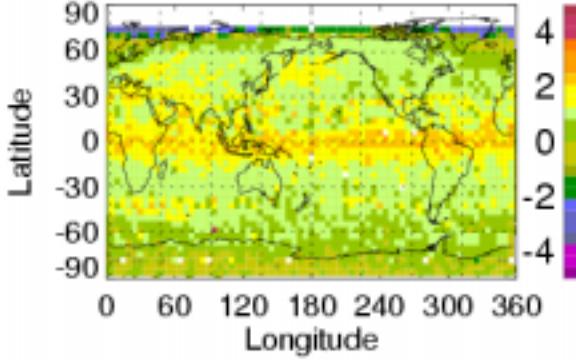
WACCM



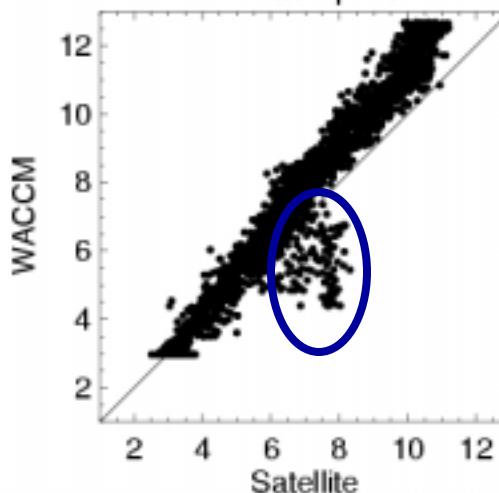
Satellite (4x5)



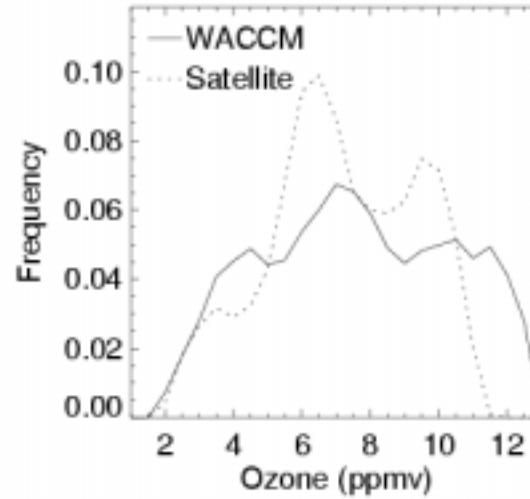
WACCM-Satellite



Scatterplot



PDFs

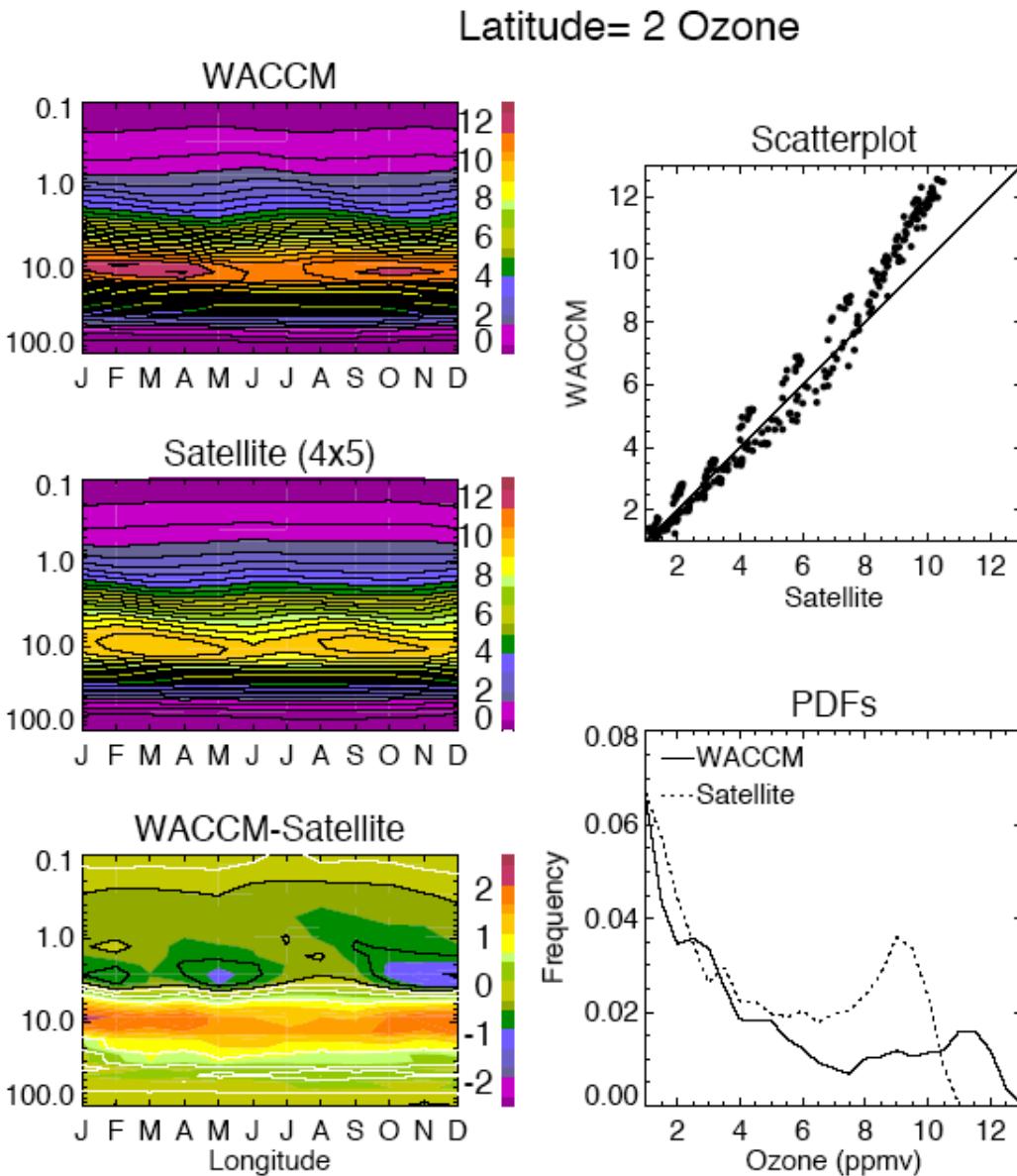


Ozone Comparison with Occultation Climatology

L. Harvey and C. Randall,
LASP

Ozone Comparison with Occultation Climatology

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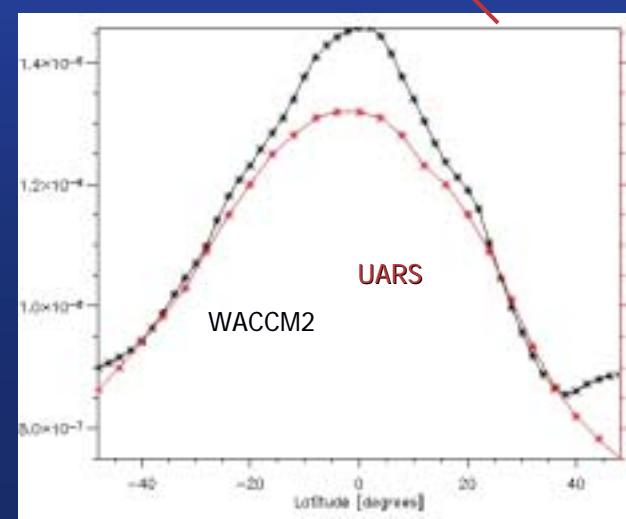
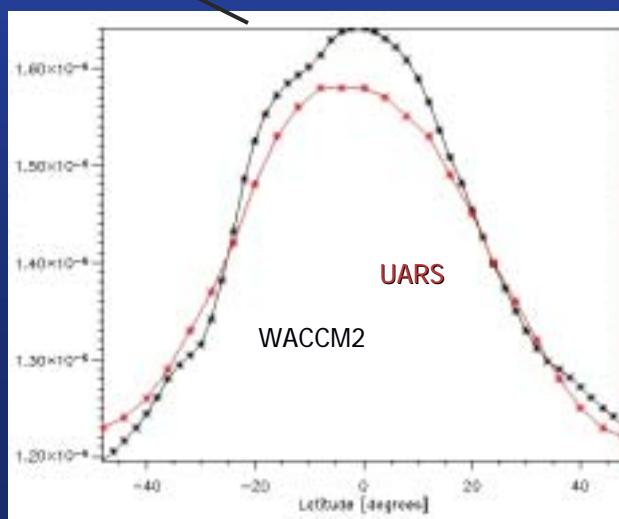
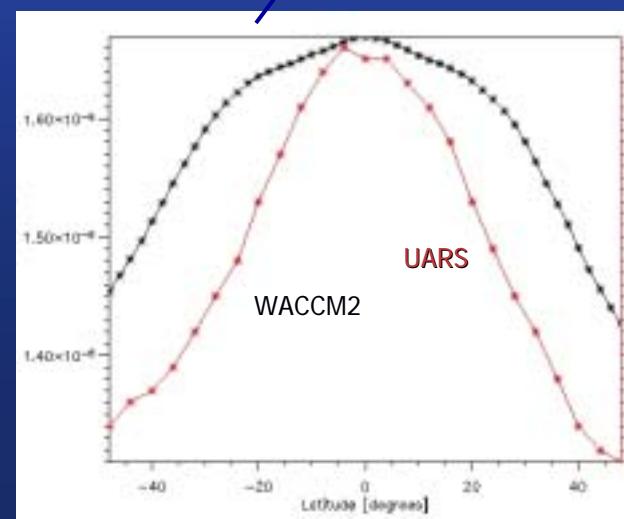
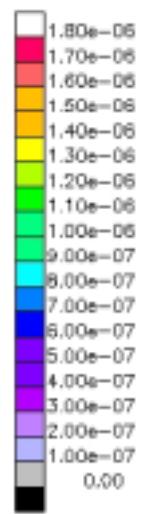
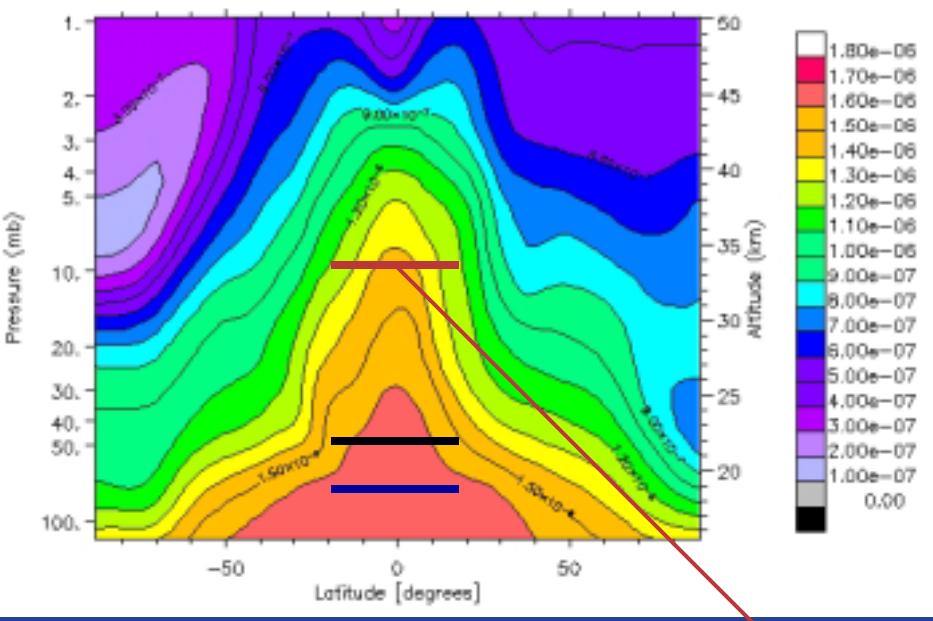
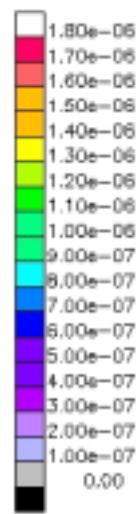
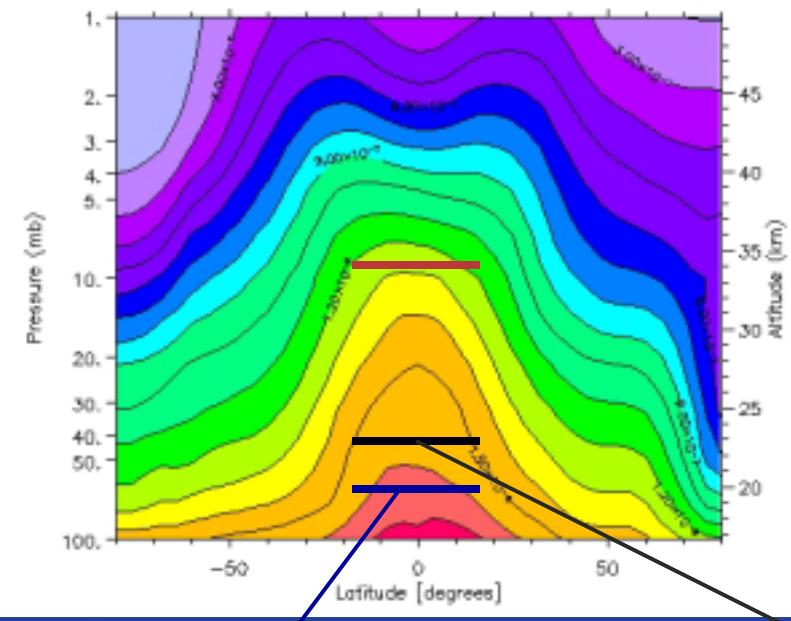


CH₄

CH₄ , April

HALOE+CLAES Clim (Courtesy of B. Randel)

WACCM2



UARS

UARS

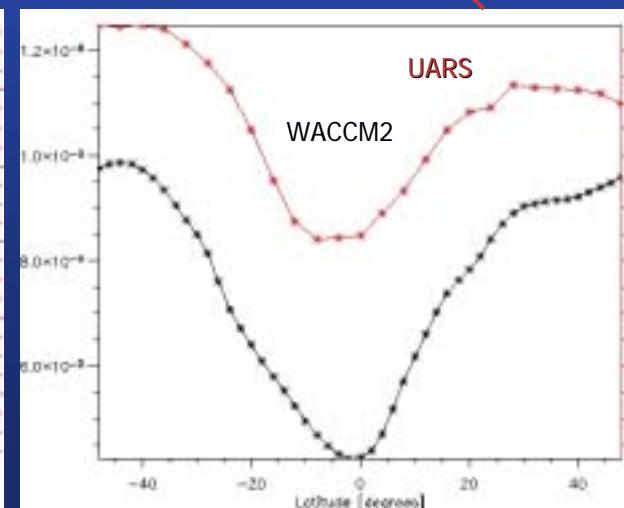
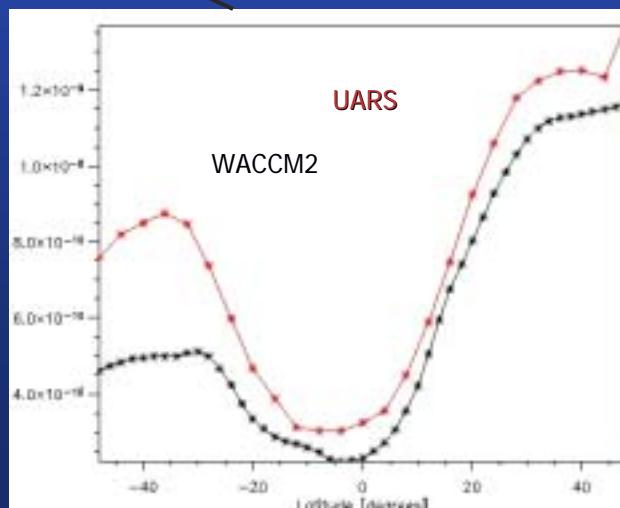
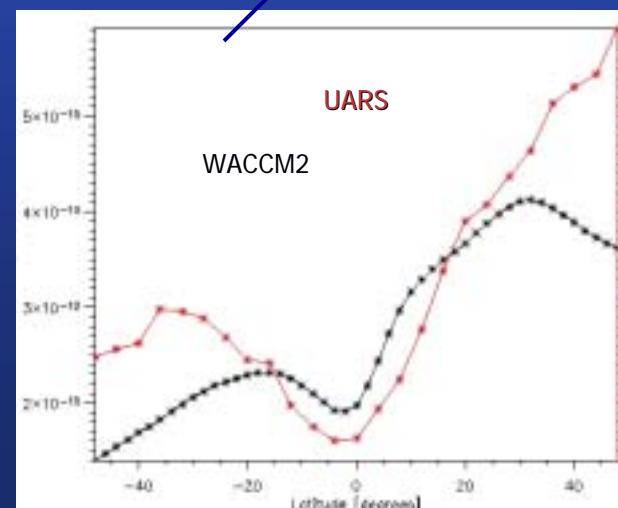
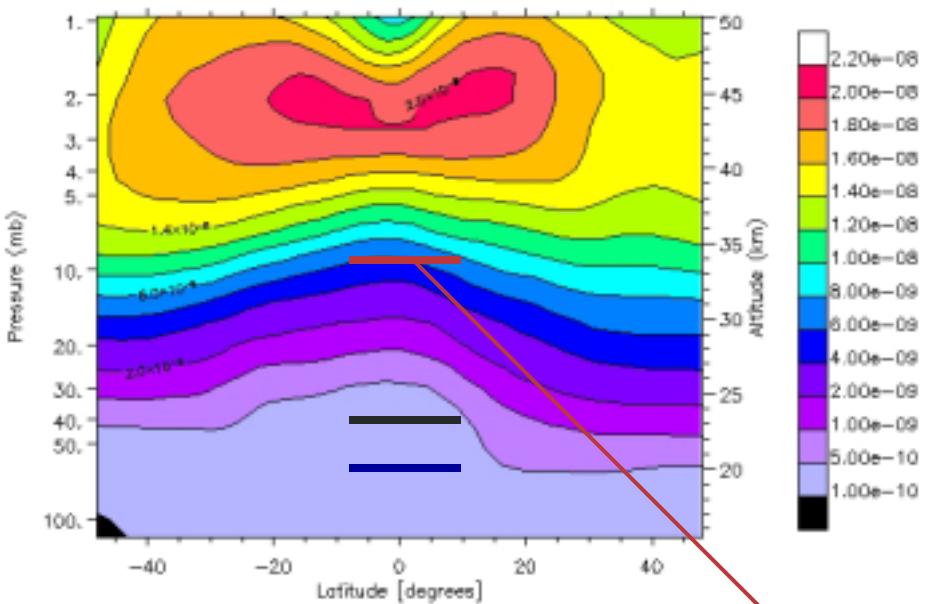
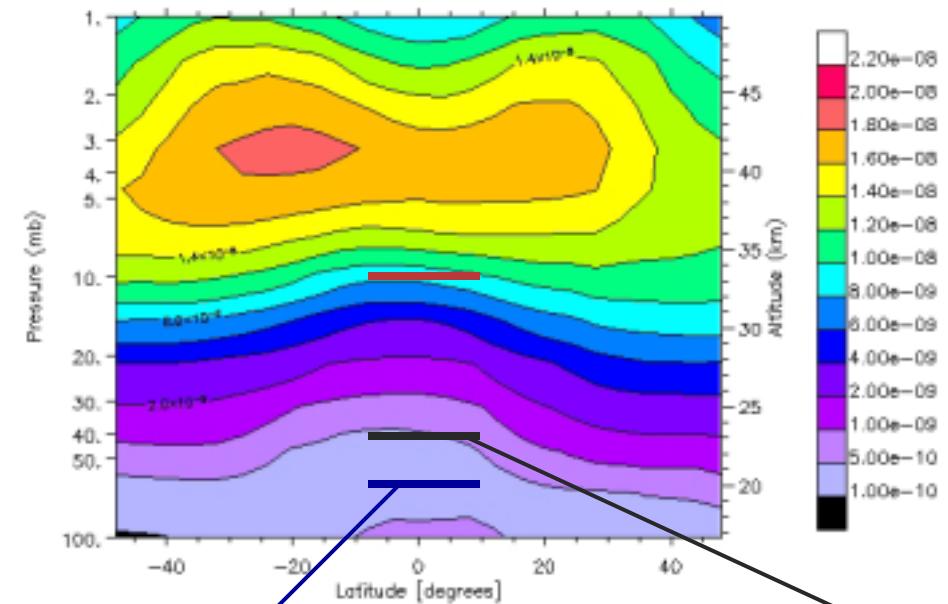
UARS

NO_x (NO+NO₂)

NO_x , April

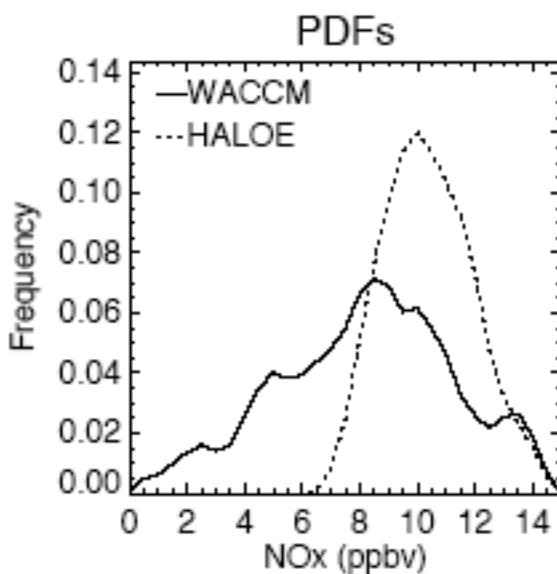
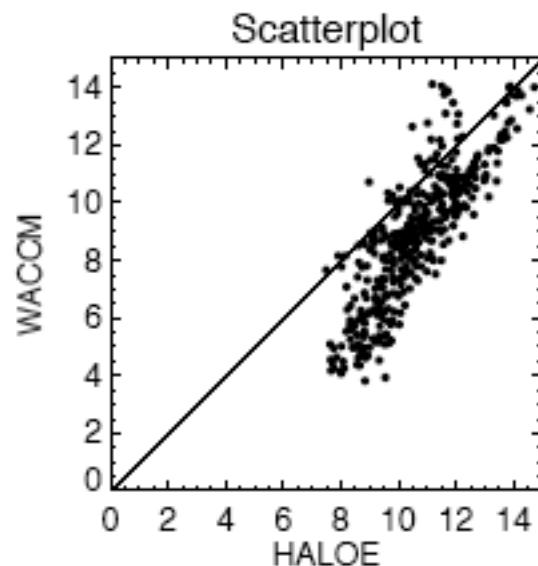
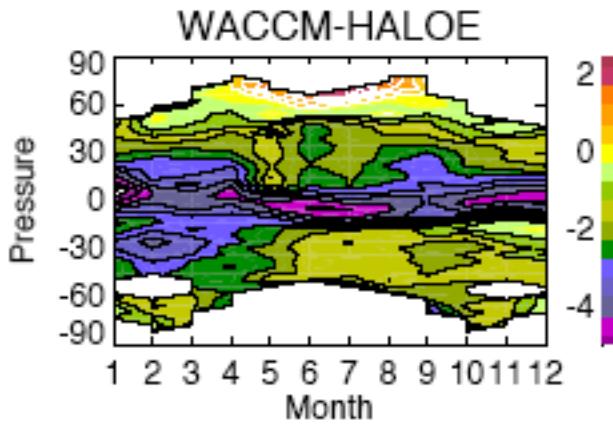
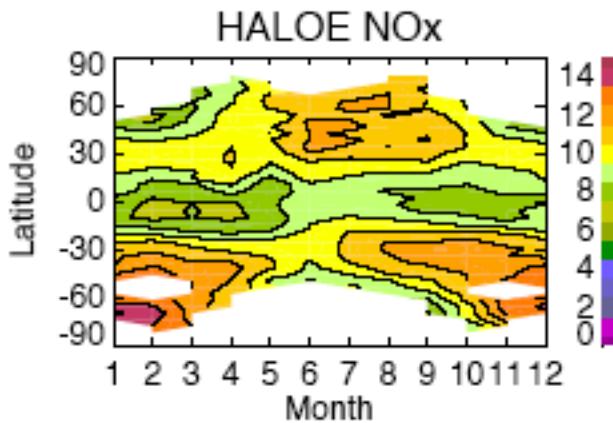
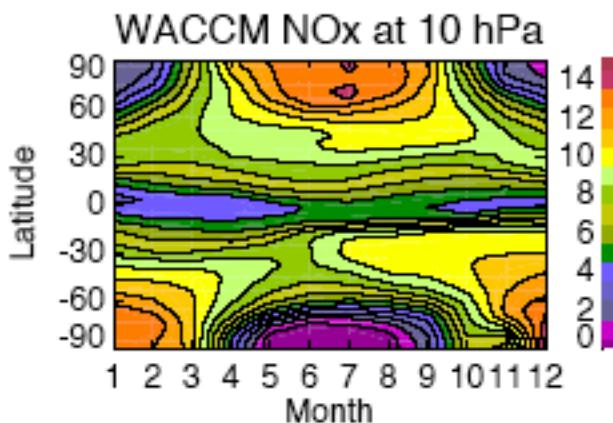
HALOE Clim. (Courtesy of B. Randel)

WACCM2



NO_x

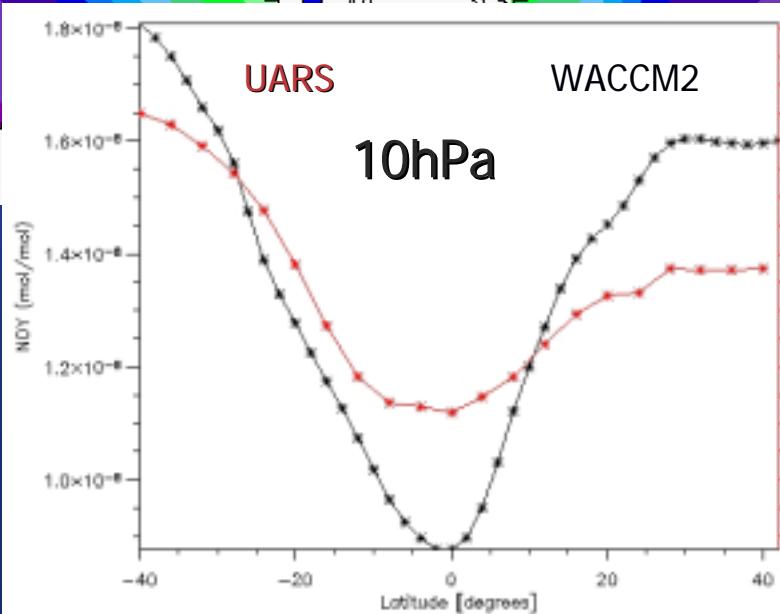
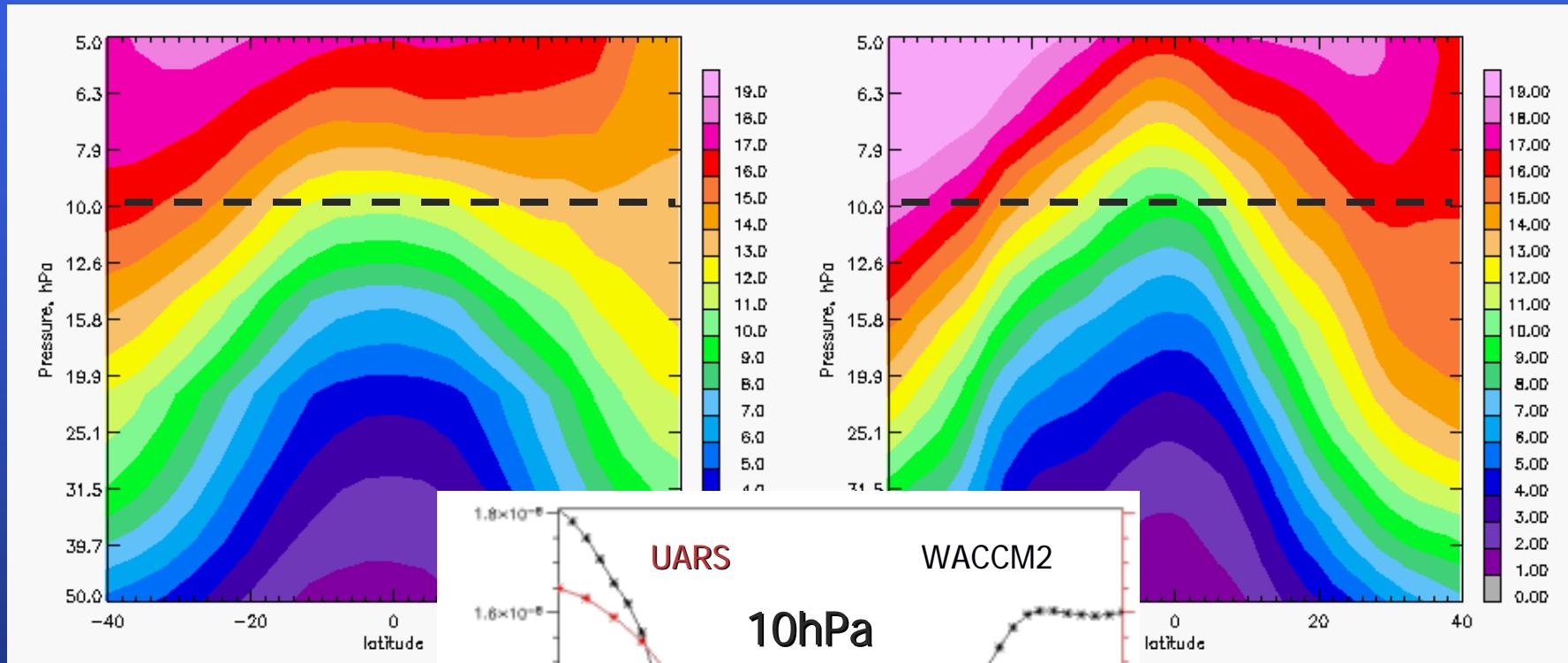
L. Harvey and C.
Randall, LASP



NO_x, April, Monthly Mean

UARS: NO_x HALOE+ HNO₃ CLAES

WACCM2



HNO₃

HNO₃

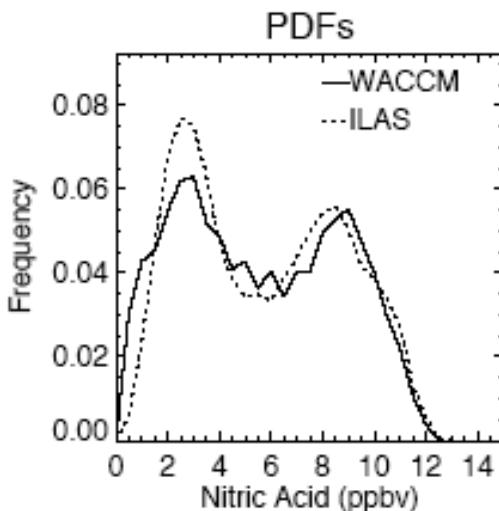
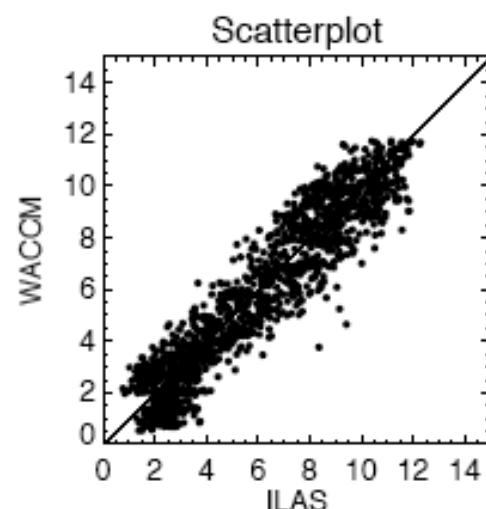
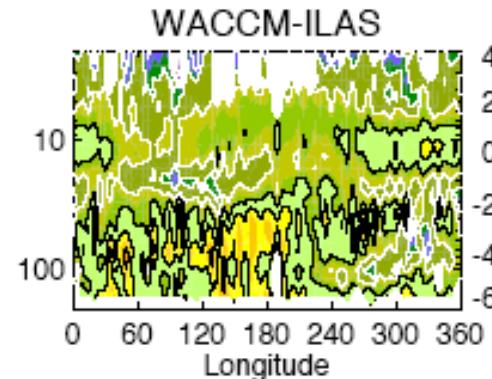
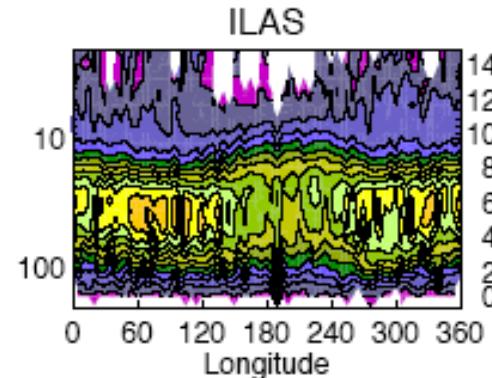
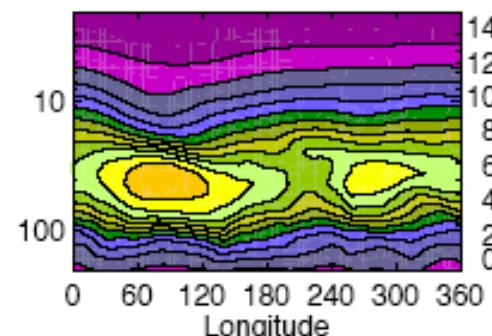
66°N

February

Late Winter

February 66deg Nitric Acid

WACCM



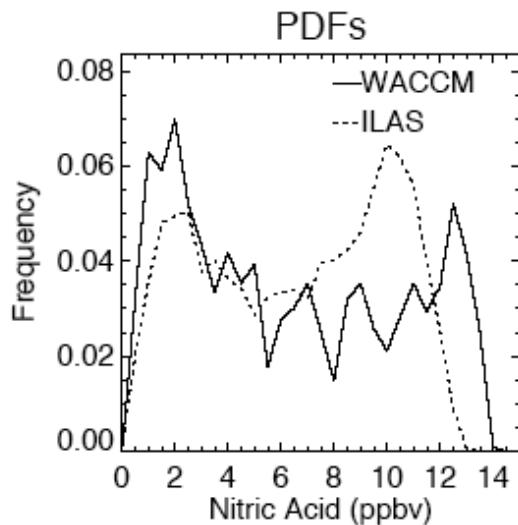
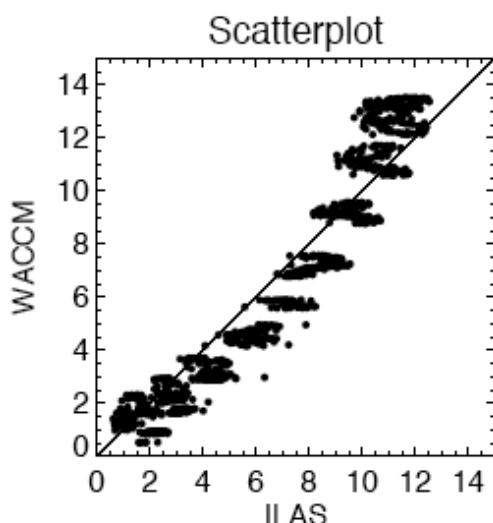
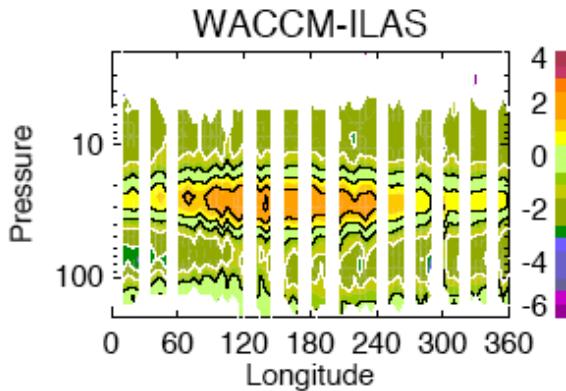
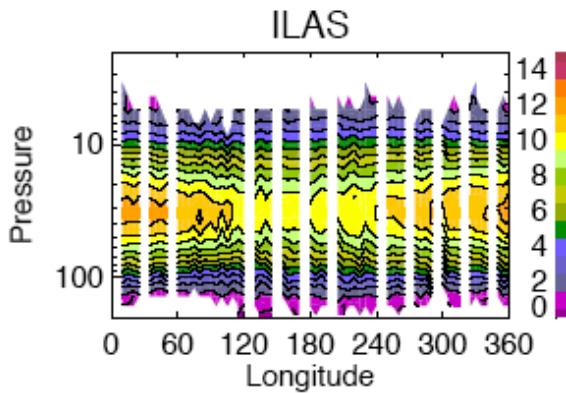
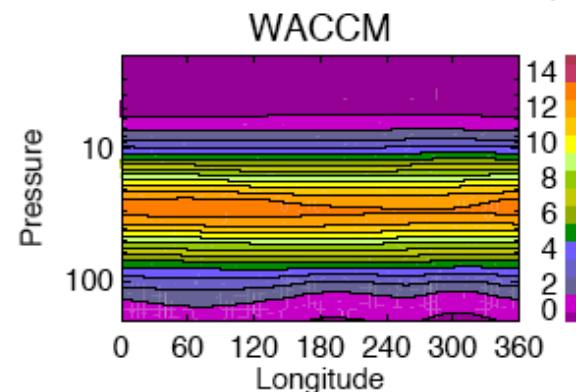
HNO_3

82°S

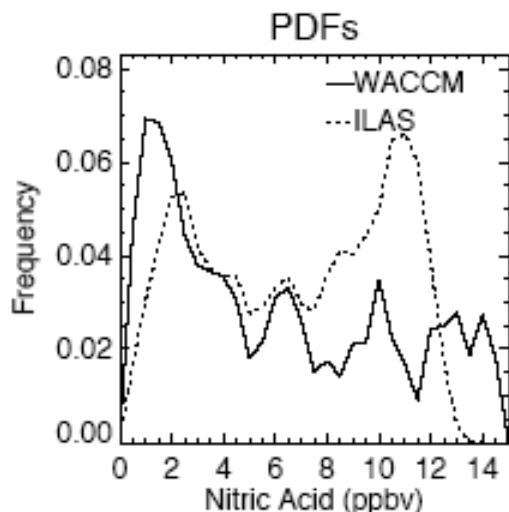
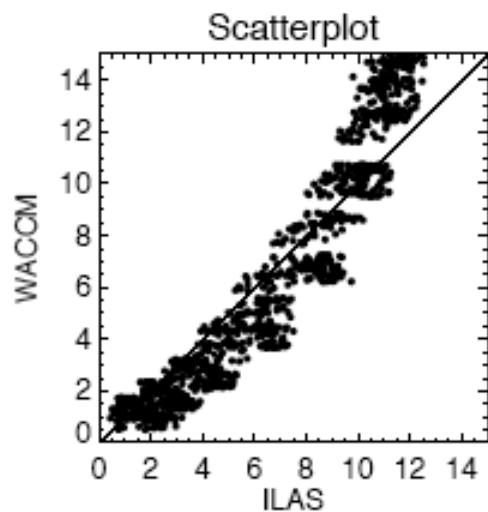
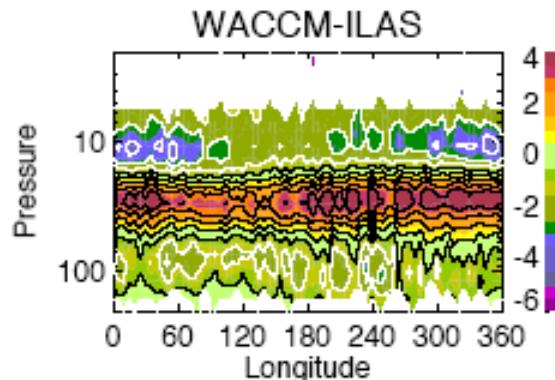
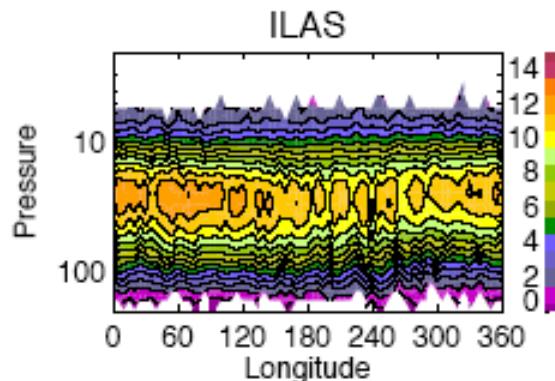
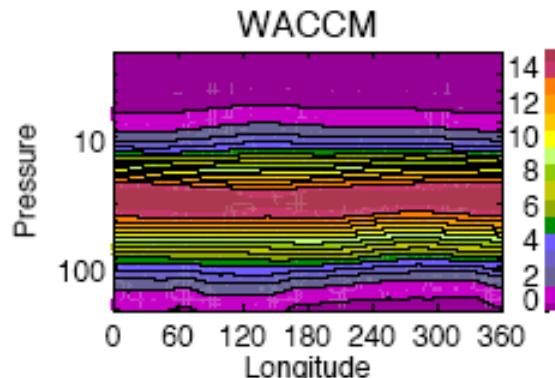
April

Fall

April -82deg Nitric Acid



May -74deg Nitric Acid

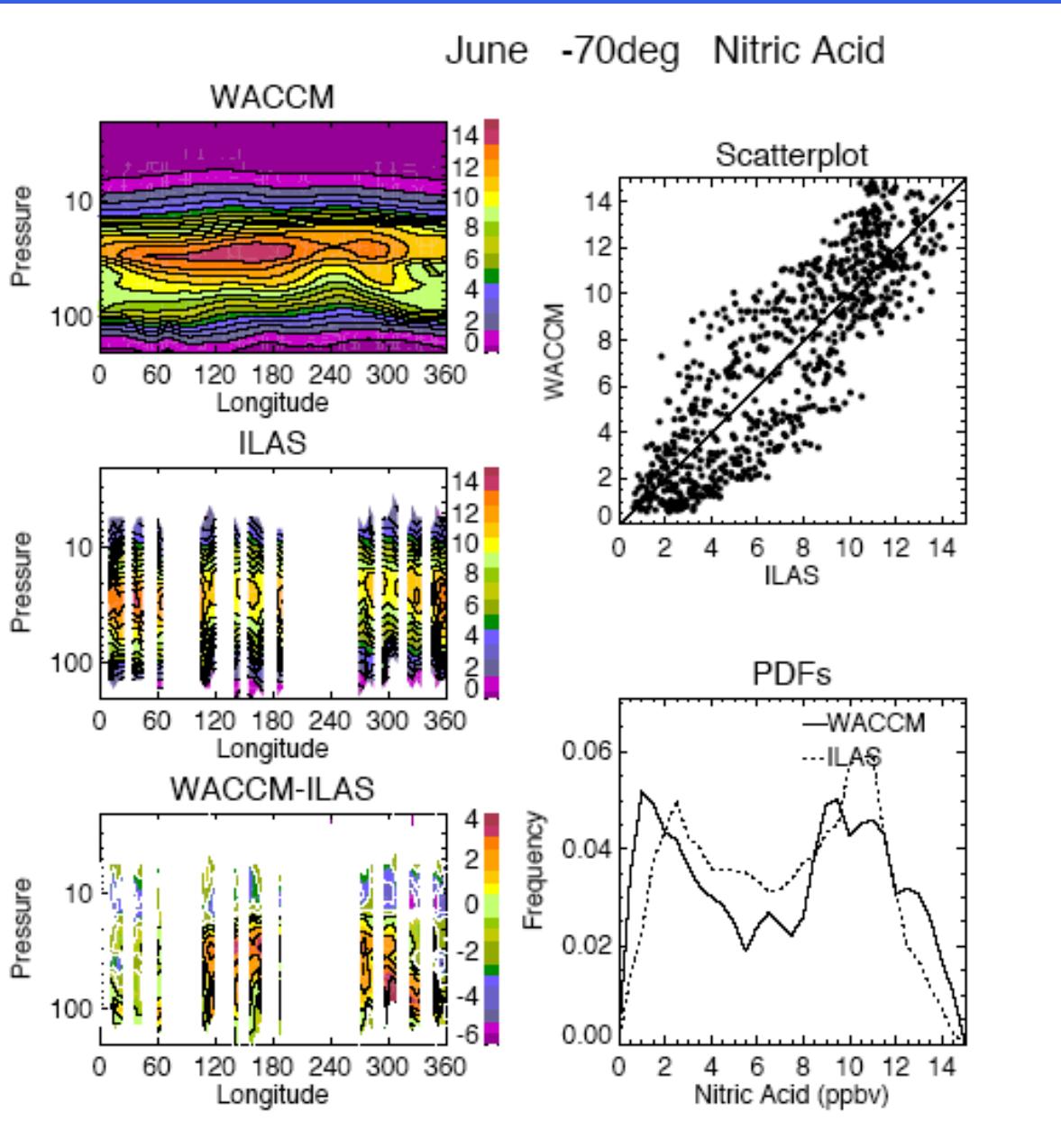


HNO₃

74°S

May

Late Fall



HNO₃
70°S
June
Early Winter

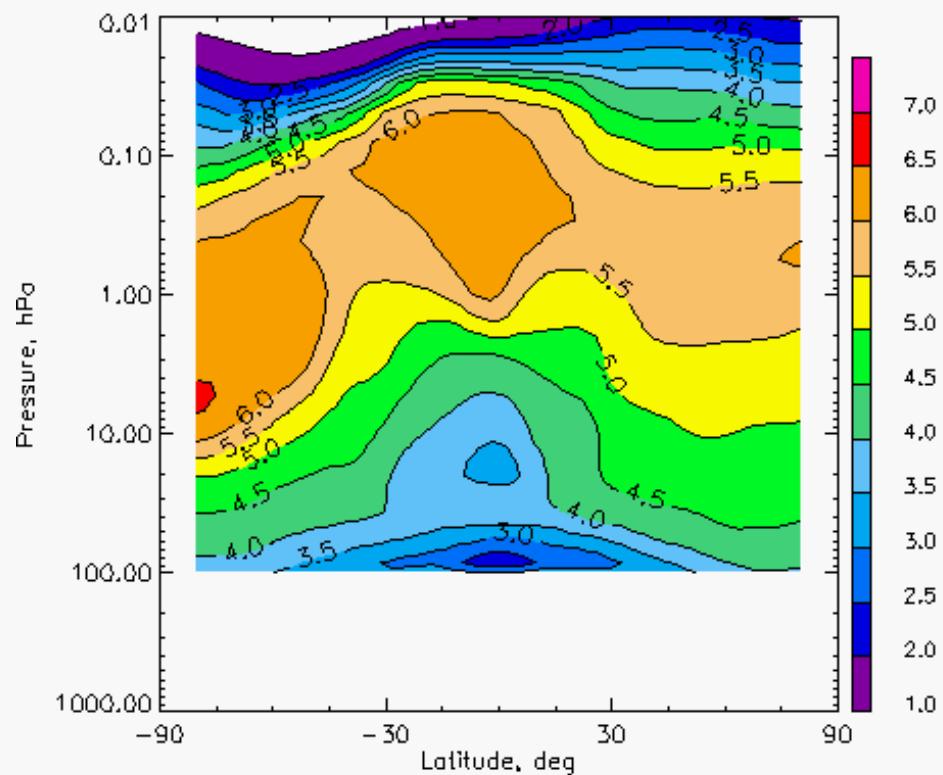
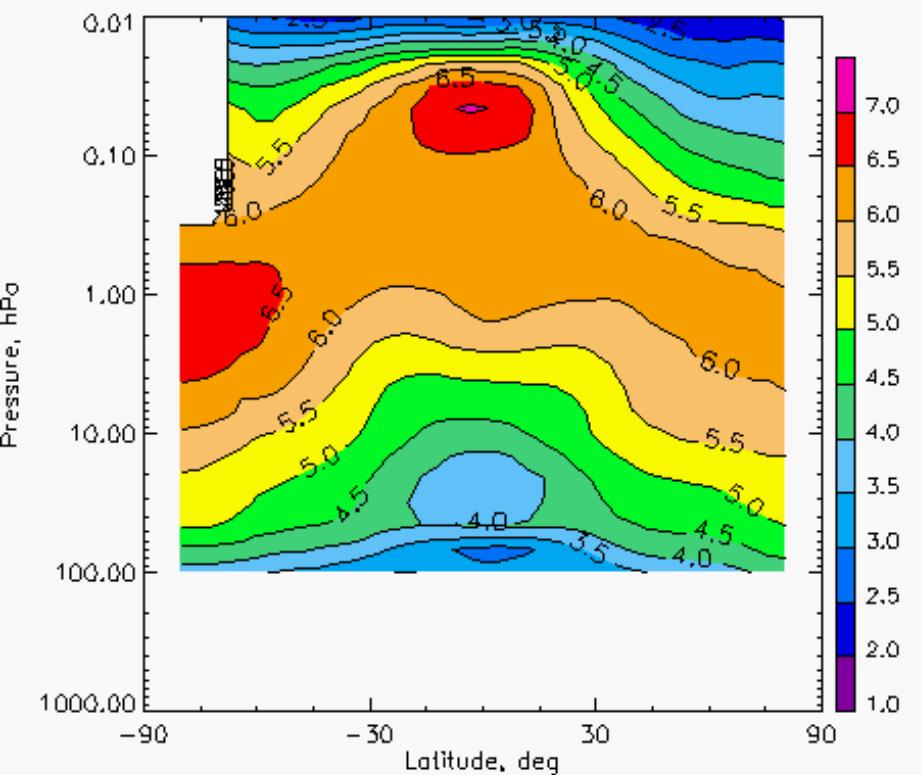
H₂O

H_2O (WACCM2)

Stratosphere / Mesosphere Distribution *** May

HALOE/MLS

WACCM2



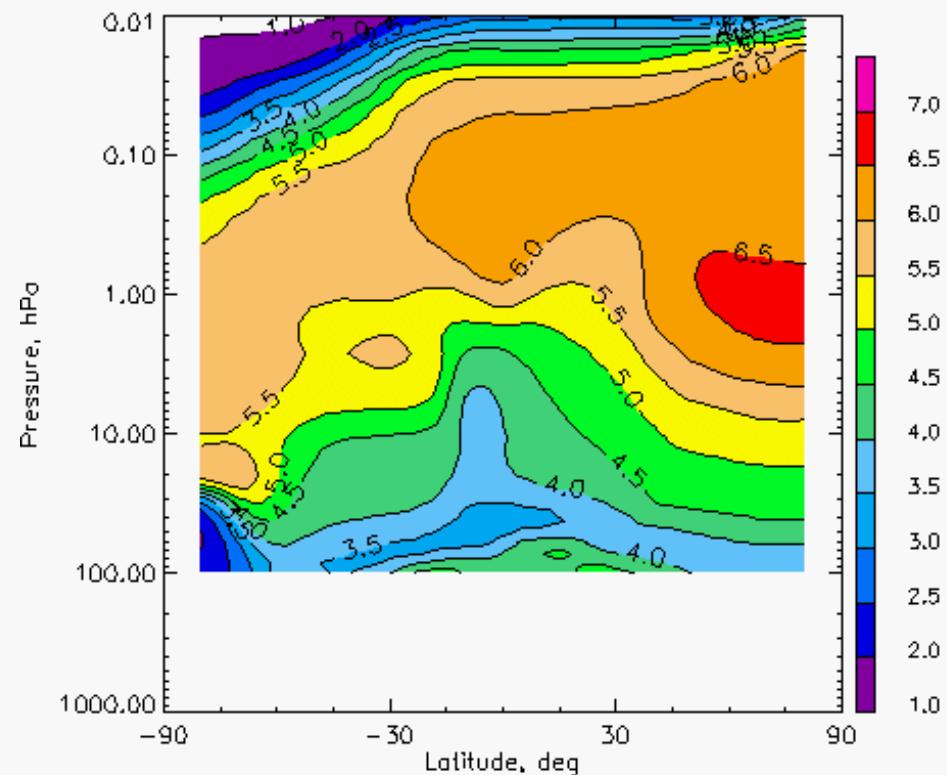
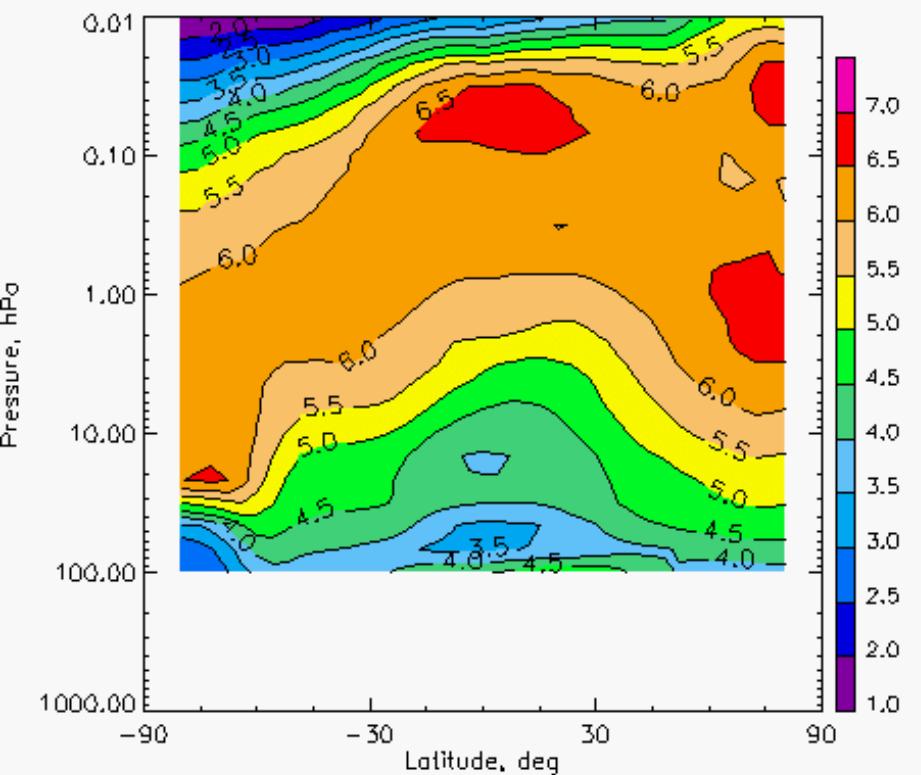
Randel et al., JGR, 2001

H_2O (WACCM2)

Stratosphere / Mesosphere Distribution *** September

HALOE/MLS

WACCM2

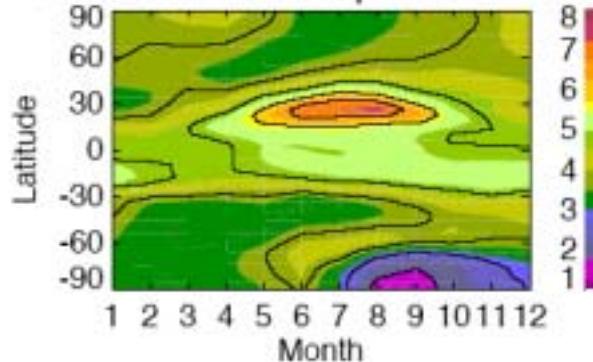


Randel et al., JGR, 2001

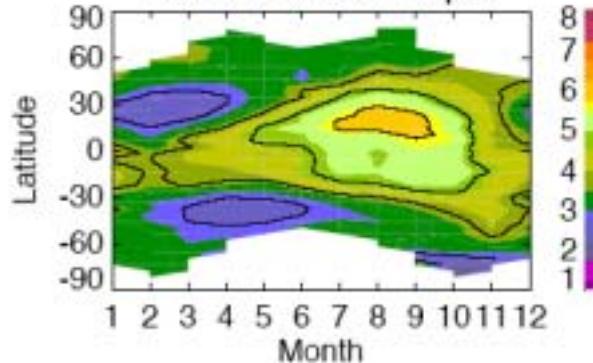
H_2O (ppmv)

118 hPa

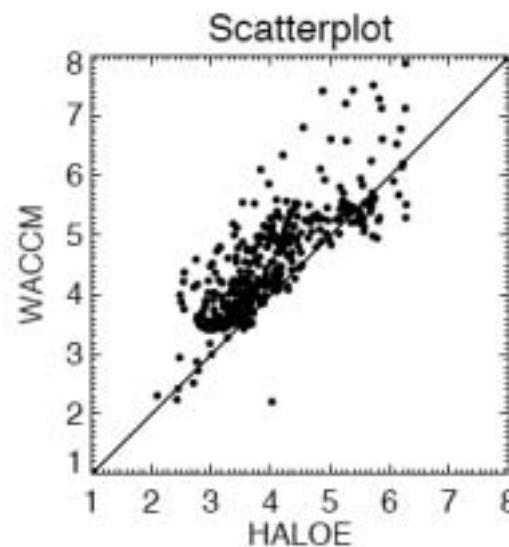
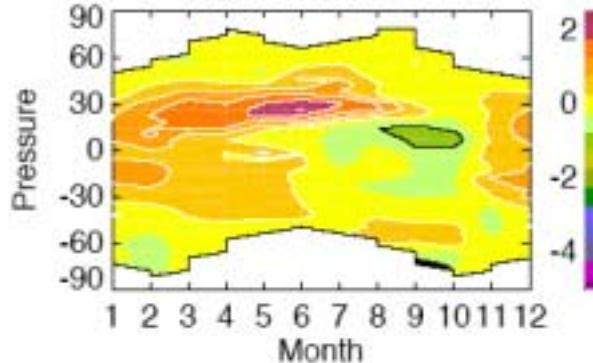
WACCM Water Vapor at 118 hPa



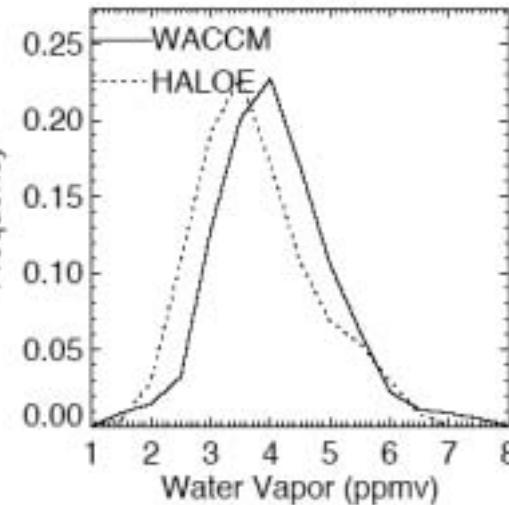
HALOE Water Vapor



WACCM-HALOE



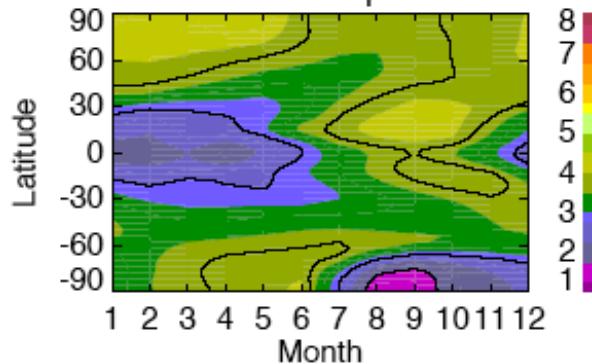
PDFs



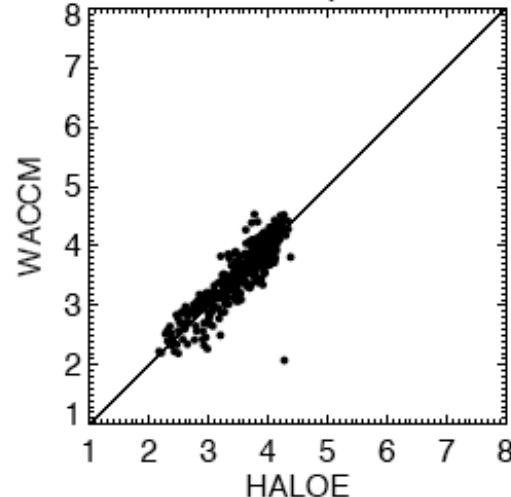
H_2O (ppmv)

85 hPa

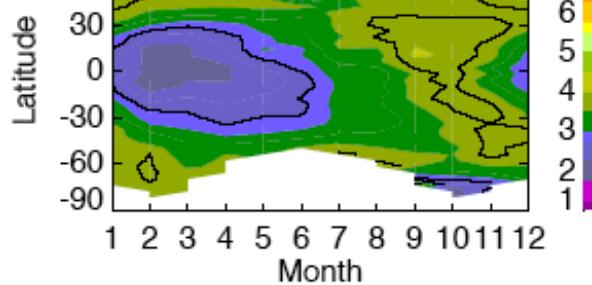
WACCM Water Vapor at 85 hPa



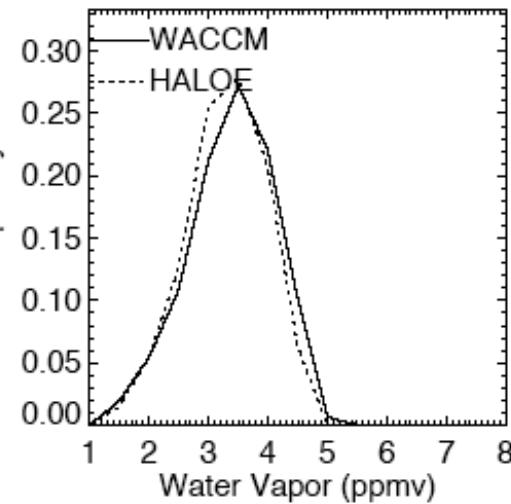
Scatterplot



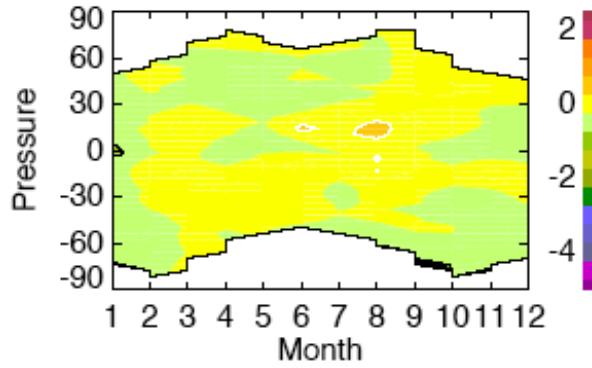
HALOE Water Vapor



PDFs

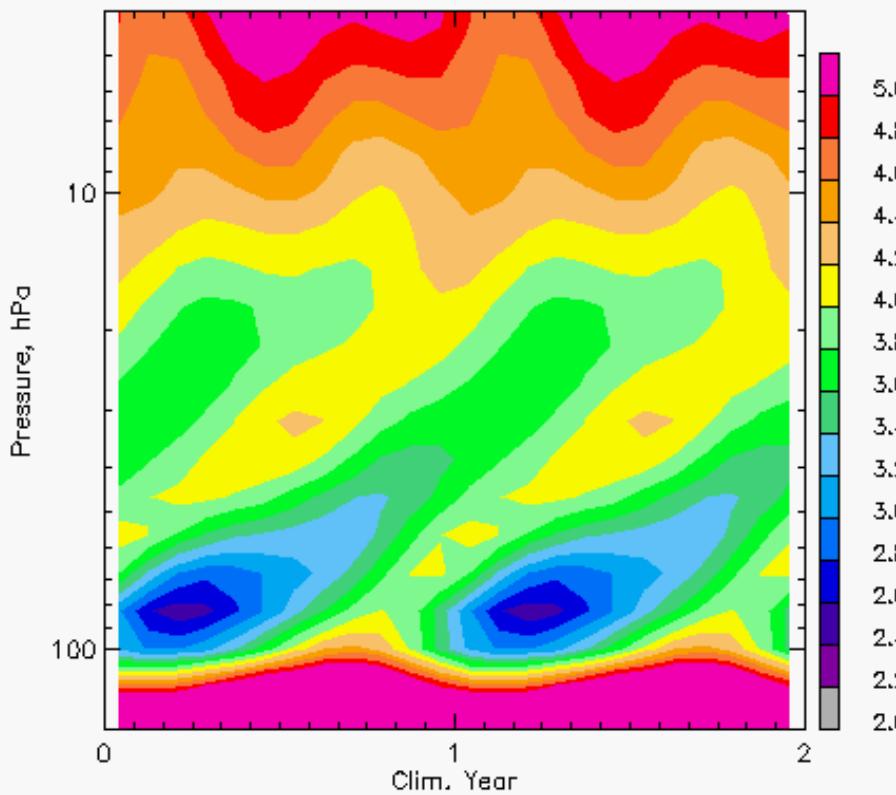


WACCM-HALOE

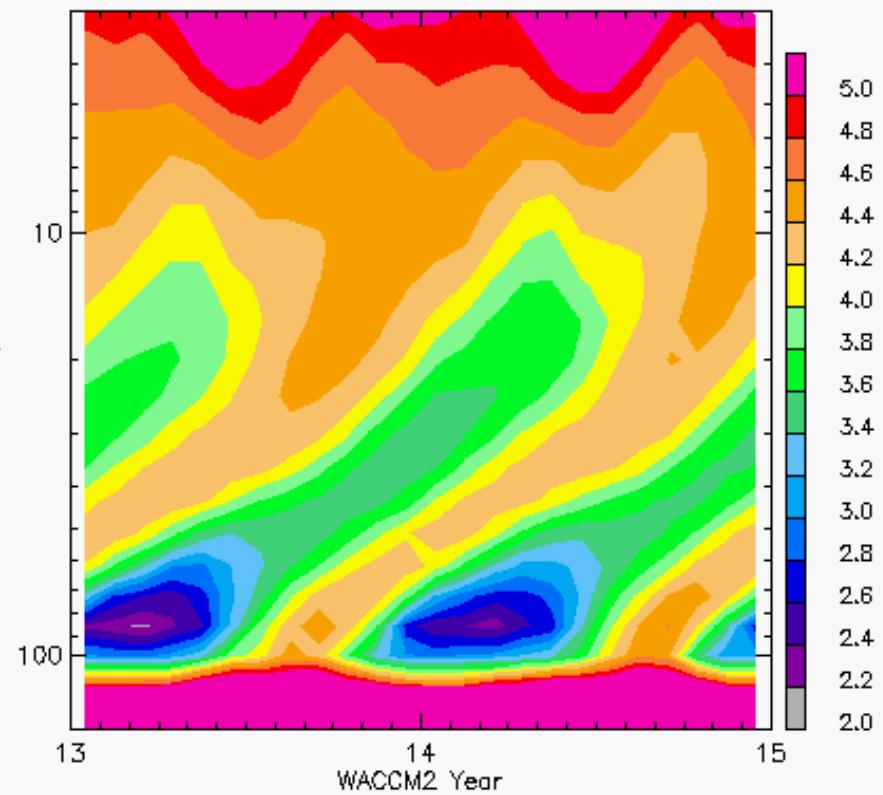


H_2O - Tape Recorder, EQ Region, ZM

HALOE



WACCM2



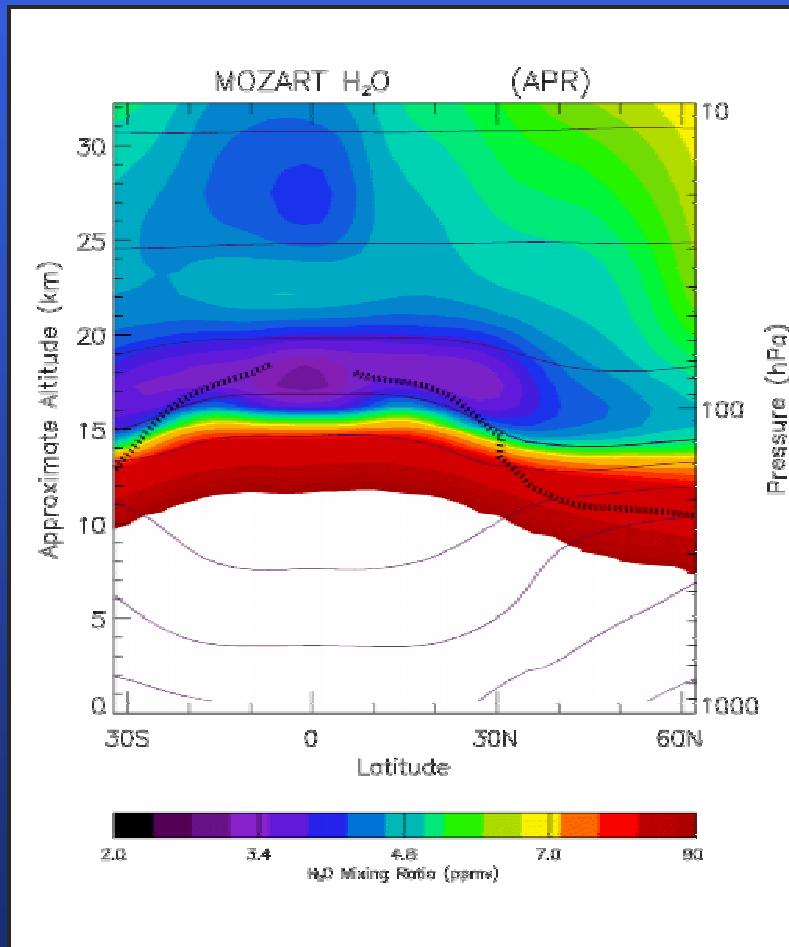
Randel et al., JGR, 2001

H₂O Movie

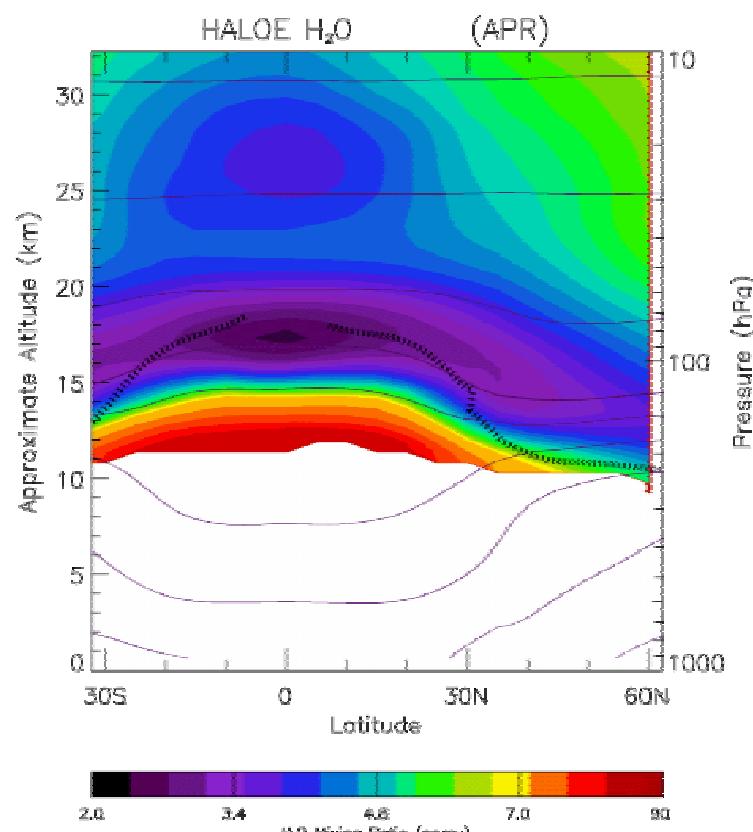
- Courtesy of Mijeong Park
- MOZART3 / WACCM1b
- Average over the South Asian Monsoon Region
 - 60° -120° E
- 30S - 60N; 0-30km
- April through March
- Model on Left; HALOE on Right.

H_2O - Tape Recorder / Monsoon Region

MOZART3/ WACCM1b

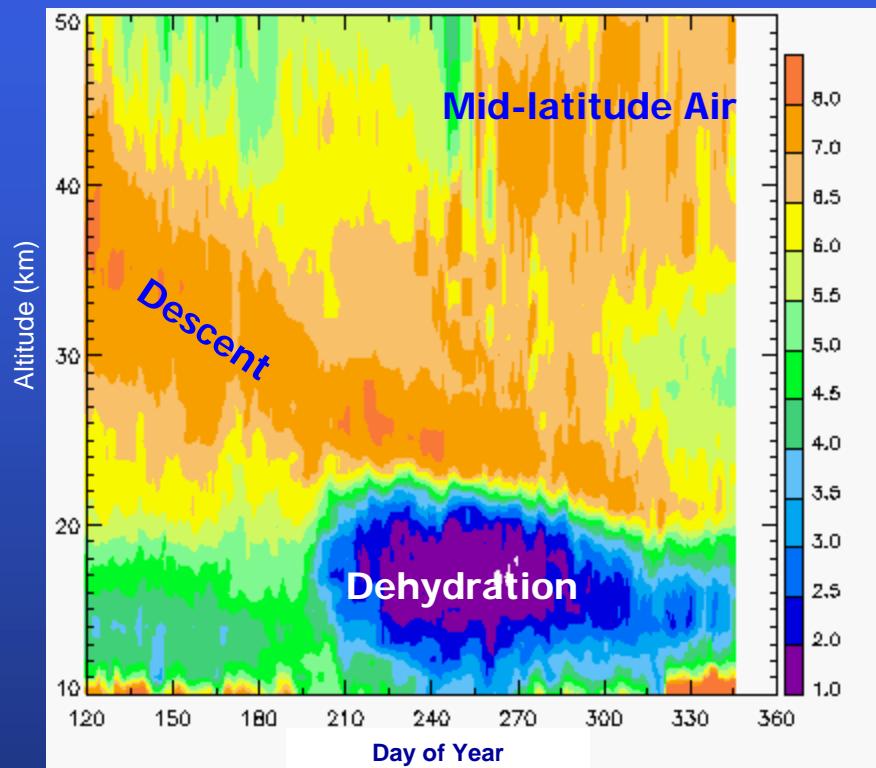


HALOE

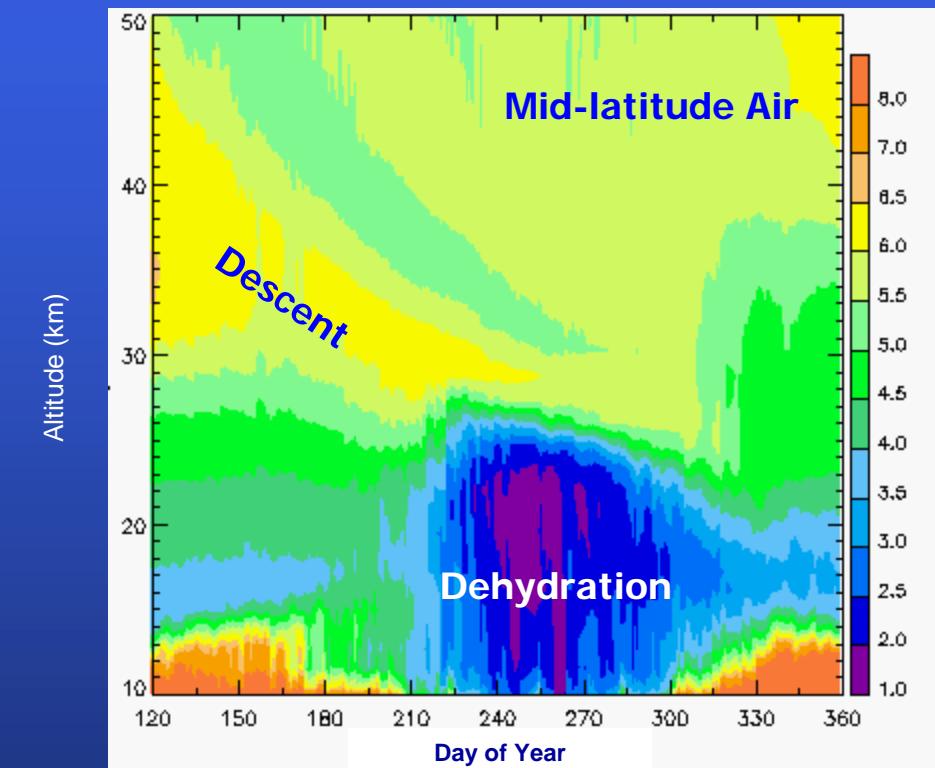


H_2O SH- Dehydration

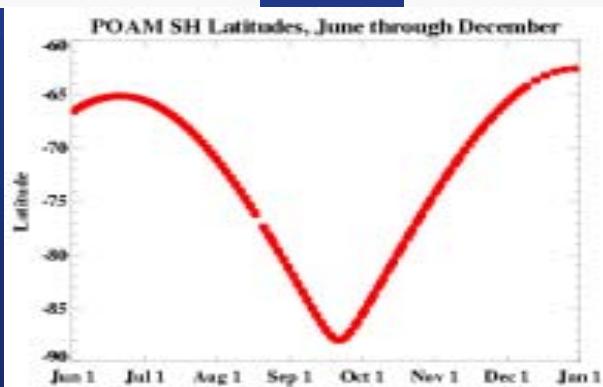
POAMIII, 1998



WACCM2 (sampled like POAMIII)



WMO 2002, Figure 3-19,
Nedoluha et al., 2000.



Describe Model Components

Evaluation with Observations

Future use of occultation data

Process Oriented Validation of Chemistry/Climate Models

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

- Sponsors: DLR / SPARC / GRIPS / PCMDI .
- Leads: Veronika Eyring (DLR), Niel Harris, Markus Rex, Ted Shepperd, D. Fahey, J. Austin, M. Dameris, H. Graf, T. Nagashima, B. Santer, R. Salawitch et al...
- Motivation: “the need to evaluate the skill of coupled chemistry-climate models to predict the future state of the ozone layer.” ... “Need to validate these processes by comparison with observations and other models”.
- SPARC Newsletter, #22, January 2004.
- <http://www.pa.op.dlr.de/workshops/ccm2003/>

The End